Lecture 16: Integral Theorems

Reading:
Kreyszig Sections: 10.8, 10.9 (pages463–467, 468–473)

Higher-dimensional Integrals

The fundamental theorem of calculus was generalized in a previous lecture from an integral over a single variable to an integration over a region in the plane. Specifically, for generalizing to Green's theorem in the plane, a vector derivative of a function integrated over a line and evaluated at its endpoints was generalized to a vector derivative of a function integrated over the plane.

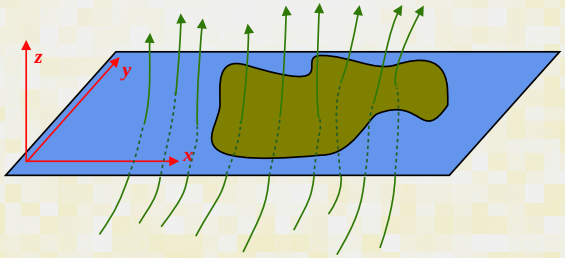

Figure 16-14: Illustrating how Green's theorem in the plane works. If a *known* vector function is integrated over a region in the plane then that integral should only depend on the bounding curve of that region.

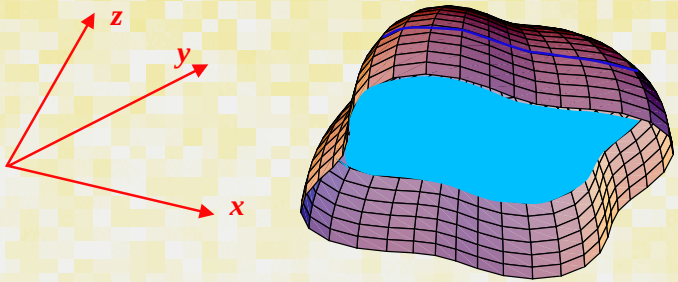

Figure 16-15: Illustration of a generalization to the Green's theorem in the plane: Suppose there is a bowl of a known shape submerged in a fluid with a trapped bubble. The bubble is bounded by two different surfaces, the bowl down to $z = 0$ and the planar liquid surface at that height. Integrating the function $\int_{V_B} dV$ over the bubble gives its volume. The volume must also be equal to an integral $\int \int_{\partial V_B} z dx dy$ over the (oriented) surface of the liquid. However, the volume of bubble can be determined from only the curve defined by the intersection of the bowl and the planar liquid surface; so the volume must also be equal to $\oint_C (\text{some function}) ds$.

The Divergence Theorem

Suppose there is "stuff" flowing from place to place in three dimensions.

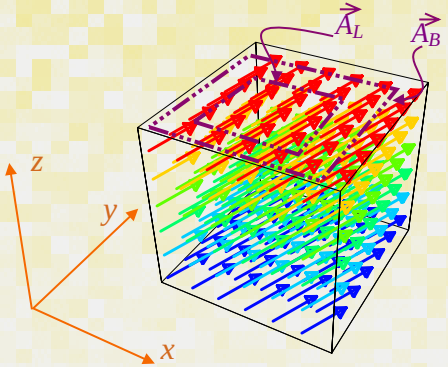

Figure 16-16: Illustration of a vector "flow field" $\vec{J}$ near a point in three dimensional space. If each vector represents the rate of "stuff" flowing per unit area of a plane that is normal to the direction of flow, then the dot product of the flow field integrated over a planar oriented area $\vec{A}$ is the rate of "stuff" flowing through that plane. For example, consider the two areas indicated with purple (or dashed) lines. The rate of "stuff" flowing through those regions is $\vec{J} \cdot \vec{A_B} = \vec{J} \cdot \hat{k} A_B$ and $\vec{J} \cdot \vec{A_L} = \vec{J} \cdot \hat{k} A_L$.

If there are no sources or sinks that create or destroy stuff inside a small box surrounding a point, then the change in the amount of stuff in the volume of the box must be related to some integral over the box's surface:

$$\begin{aligned} \frac{d}{dt}(\text{amount of stuff in box}) &= \frac{d}{dt}\int_{\text{box}} (\frac{\text{amount of stuff}}{\text{volume}}) dV \\ &= \int_{\text{box}} \frac{d}{dt}(\frac{\text{amount of stuff}}{\text{volume}}) dV \\ &= \int_{\text{box}} (\text{some scalar function related to } \vec{J}) dV \\ &= \int_{\substack{\text{box} \\ \text{surface}}} \vec{J} \cdot d\vec{A} \end{aligned} \tag{16-1}$$

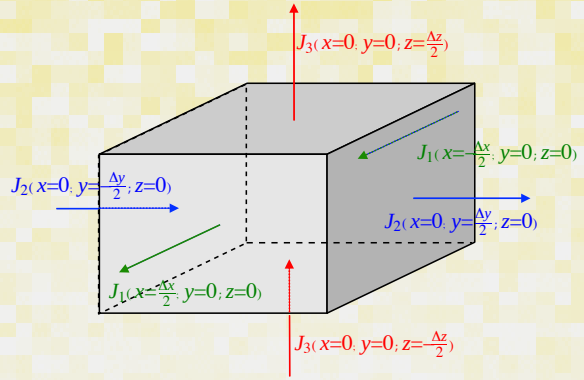

Figure 16-17: Integration of a vector function near a point and its relation to the change in that vector function. The rate of change of stuff is the integral of flux over the outside—and in the limit as the box size goes to zero, the rate of change of the amount of stuff is related to the sum of derivatives of the flux components at that point.

To relate the rate at which "stuff M" is flowing into a small box of volume $\delta V = dxdydz$ located at (x, y, z) due to a flux $\vec{J}$, note that the amount that M changes in a time Δt is:

$$\begin{aligned}\Delta M(\delta V) &= (M \text{ flowing out of } \delta V) - (M \text{ flowing in } \delta V) \\ &= \vec{J}(x-\tfrac{dx}{2})\hat{i}dydz - \vec{J}(x+\tfrac{dx}{2})\cdot\hat{i}dydz \\ &+ \vec{J}(y-\tfrac{dy}{2})\hat{j}dzdx - \vec{J}(y+\tfrac{dy}{2})\cdot\hat{j}dzdx \;\; \Delta t \\ &+ \vec{J}(z-\tfrac{dz}{2})\hat{k}dxdy - \vec{J}(z+\tfrac{dz}{2})\cdot\hat{k}dxdy \\ &= -(\frac{\partial J_x}{\partial x}+\frac{\partial J_y}{\partial y}+\frac{\partial J_z}{\partial z})\delta V\Delta t + \mathcal{O}(dx^4)\end{aligned} \tag{16-2}$$

If $C(x, y, z) = M(\delta V)/\delta V$ is the concentration (i.e., stuff per volume) at (x, y, z), then in the limit of small volumes and short times:

$$\frac{\partial C}{\partial t} = -(\frac{\partial J_x}{\partial x}+\frac{\partial J_y}{\partial y}+\frac{\partial J_z}{\partial z}) = -\nabla\cdot\vec{J} = -\text{div}\vec{J} \tag{16-3}$$

For an arbitrary closed volume V bounded by an oriented surface ∂V:

$$\frac{dM}{dt} = \frac{d}{dt}\int_V C dV = \int_V \frac{\partial C}{\partial t} dV = -\int_V \nabla \cdot \vec{J} dV = -\int_{\partial V} \vec{J} \cdot d\vec{A} \tag{16-4}$$

The last equality

$$\int_V \nabla \cdot \vec{J} dV = \int_{\partial V} \vec{J} \cdot d\vec{A} \tag{16-5}$$

is called the Gauss or the divergence theorem.

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London Dispersion Interaction between a point and Closed Volume

notebook (non-evaluated) pdf (evaluated) html (evaluated)

If the London interaction (i.e., energy between two induced dipoles) can be treated as a $1/r^6$ potential, then the potential due to a volume is an integration over each point in the volume and and arbitrary point in space. This calculation will be made much more efficient by turning the volume integral into a surface integral by using the divergence theorem.

1: To find a vector potential, $\vec{F}$ which has a divergence that is equal to $\nabla \cdot \vec{F} = -1/\|\vec{r} - \vec{x}\|^6$, *FVecLondon* is a 'guess.'

3: Using `Div` in the `Calculus`VectorAnalysis`` package, this will show that the guess *FVecLondon* is a correct vector function for the $1/r^6$ potential.

6: This will be the multiplier elemental area for a parameterized cylindrical surface $|d\vec{r}/d\theta \times d\vec{r}/dz|$.

7: *CylinderIntegrandθζ* is the integrand which would apply on a cylindrical surface.

8: This attempt to integrate *CylinderIntegrandθζ* over θ does not result in a closed form.

9: However, integrating *CylinderIntegrandθζ* over z does produce a closed form that could be subsequently integrated over θ numerically.

Find $\vec{F}$ such that div $\vec{F}$ is $\frac{-1}{(\vec{r}-\vec{x})^6}$ where $\vec{r}$ = (ξ,η,ζ) is a position in the cylinder and $\vec{x}$=(x,y,z) is a general position in space

The following is a ``guess'' at the vector potential; it will be verified as the correct one by checking its divergence.

```
1 FVecLondon = 1/(3((ξ-x)^2+(η-y)^2+(ζ-z)^2)^3) {ξ-x, η-y, ζ-z}
2 << Calculus`VectorAnalysis`
3 FullSimplify[Div[FVecLondon, Cartesian[ξ, η, ζ]]]
```

Cylinder Surface normals and differential quantities

```
4 CylSurf = {R Cos[t], R Sin[t], ζ}
5 CylSurfRt = D[CylSurf, t]
  CylSurfRz = D[CylSurf, ζ]
6 NormalVecCylSurf = Cross[CylSurfRt, CylSurfRz]
7 CylinderIntegrandθζ =
    FullSimplify[(FVecLondon /. {ξ → R Cos[t], η → R Sin[t]}).
      NormalVecCylSurf]
8 Integrate[CylinderIntegrandθζ, t,
    Assumptions -> R > 0 && ζ ∈ Reals &&
      x ∈ Reals && y ∈ Reals && z ∈ Reals]
9 CylinderIntegrandθInd ζ = Integrate[CylinderIntegrandθζ, ζ,
    Assumptions -> R > 0 && L > 0 && x ∈ Reals &&
      y ∈ Reals && z ∈ Reals && t ∈ Reals]
```

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Efficiency and Speed Issues: When to Evaluate the Right-Hand-Side of a Function in MATHEMATICA® .

The standard practice is to define functions in mathematica with `:=`. However, sometimes it makes sense to evaluate the right-hand-side when the function definition is made. These are the cases where the right hand side would take a long time to evaluate—each time the function is called, the evaluation would be needed again and again. The following example illustrates a case where it makes sense to use `Evaluate` in a function definition (or, equivalently defining the function with immediate assignment `=`).

To Evaluate or Not to Evaluate when Defining Functions

notebook (non-evaluated) pdf (evaluated) html (evaluated)

This example illustrates a case in which immediate evaluation `=` would be preferable to delayed evaluation `:=`

```
1  Timing[Integrate[Exp[Tan[x]], {x, 0, c}]]
2  Timing[Integrate[Exp[Tan[x]], {x, 0, c}]]
3  Timing[f[c_] := Evaluate[Integrate[Exp[Tan[x]], {x, 0, c}]]]
4  Timing[h[c_] = Integrate[Exp[Tan[x]], {x, 0, c}]]
5  Timing[g[c_] := Integrate[Exp[Tan[x]], {x, 0, c}]]
6  ?f
7  ?h
8  ?g
9  Timing[f[0.5]]
10 Timing[h[0.5]]
11 Timing[g[0.5]]
```

1: When a non-trivial integral is done for the first time, Mathematica loads various libraries. Notice the difference in timing between this first computatation of $\int \exp[\tan(x)]dx$ and the following one.

2: The second evaluation is faster. Now, a baseline time has been established for evaluating this integral symbolically.

3: Here, to make a function definition for the integral, the symbolic integral is obtained and so the function definition *takes longer*.

4: Using an `=` is roughly equivalent to using `Evaluate` above and the time to make the function assignment should be approximately the same.

5: Here, the symbolic integration is delayed until the function is called (later). Therefore, the function assignment is very rapid.

6: The functions, where the right-hand-side was immediately evaluated, contain the symbolic information. Therefore, when the function is called later, the symbolic integration will not be needed.

8: The function with the completely delayed assignment does not have the symbolic information.

10: The speed of the function is much faster in the case where the symbolic integration is not needed.

11: The relatively slow speed of this function indicates that it would be a poor choice when numerical efficiency is an issue.

London Dispersion Potential of a Finite Cylinder

notebook (non-evaluated) pdf (evaluated) html (evaluated)

The example of using the divergence theorem to compute a $1/r^6$ potential by pushing a volume integral onto its bounding surface is continued for the particular case of a cylinder.

1: Here, `Evaluate` is used to store the result of the `Simplify` function after the bounds of the integrated function are evaluated. The result is the integrand for the cylindrical part.

2: `NIntegrate` is required to do the remaining calculation, but instead integrating over three variables, the cylinder's contribution is reduced to a single integration. Because of polar symmetry, the problem is simplified by setting x to the total distance r and setting $y = 0$.

3: These are the surface differential quantities for the top surface of the cylinder.

4: This is the integrand for the top surface.

5: The integral over θ does not return a closed form; so here the r-integral is performed explicitely.

6: `NIntegrate` is used to do the θ-integral and here a function is defined to give the contribution due to the top surface.

10: By direct analogy to the top surface, the contribution from the bottom surface is defined as a function.

11: The total potential is obtained by adding the contribution from the cylindrical side to the top and bottom surfaces' contributions.

```
1  CylinderIntegrandθ[x_, y_, z_, CylRad_, CylLen_] :=
     Evaluate[Simplify[(CylinderIntegrandθInd𝜁 /. {𝜁 -> CylLen / 2,
           R -> CylRad}) - (CylinderIntegrandθInd𝜁 /.
         {𝜁 -> -CylLen / 2, R -> CylRad}), Assumptions ->
       CylRad > 0 && CylLen > 0 && x ∈ Reals &&
       y ∈ Reals && z ∈ Reals && t ∈ Reals]]

2  CylinderContribution[dist_, z_, CylRad_, CylLen_] :=
     NIntegrate[Evaluate[CylinderIntegrandθ[
         dist, 0, z, CylRad, CylLen], {t, 0, 2 π}]]

3  TopSurf = {r Cos[t], r Sin[t], L/2}
   TopSurfRt = D[TopSurf, t]; TopSurfRr = D[TopSurf, r]
   NormalVecTopSurf = FullSimplify[Cross[TopSurfRr, TopSurfRt]]

4  TopIntegrandθr =
     FullSimplify[(FVecLondon /. {ξ → r Cos[t], η → r Sin[t], 𝜁 → L/2}).
       NormalVecTopSurf]

5  TopIntegrandθInd r = Integrate[TopIntegrandθr, r, Assumptions →
       t ≥ 0 && L > 0 && x ∈ Reals && y ∈ Reals && z ∈ Reals]

6  TopIntegrandθ[x_, y_, z_, CylRad_, CylLen_] := Evaluate[
       Simplify[(TopIntegrandθInd r /. {r -> CylRad, L -> CylLen}) -
         (TopIntegrandθInd r /. {r -> 0, L -> CylLen})]]

7  TopContribution[dist_, zpos_, CylRad_, CylLen_] :=
     NIntegrate[Evaluate[
       TopIntegrandθ[dist, 0, zpos, CylRad, CylLen], {t, 0, 2 π}]]

8  BotSurf = {r Cos[t], r Sin[t], -L/2}
   BotSurfRt = D[BotSurf, t]; BotSurfRr = D[BotSurf, r]
   NormalVecBotSurf = FullSimplify[Cross[BotSurfRt, BotSurfRr]]
   BotIntegrandr =
     FullSimplify[(FVecLondon /. {ξ → r Cos[t], η → r Sin[t], 𝜁 → -L/2}).NormalVecBotSurf]

9  BotIntegrandθInd r = Integrate[BotIntegrandθr, r, Assumptions →
       t ≥ 0 && L > 0 && x ∈ Reals && y ∈ Reals && z ∈ Reals]

10 BotContribution[dist_, zpos_, CylRad_, CylLen_] :=
     NIntegrate[Evaluate[
       BotIntegrandθ[dist, 0, zpos, CylRad, CylLen], {t, 0, 2 π}]]

11 LondonCylinderPotential[dist_, zpos_, CylRad_, CylLen_] :=
     CylinderContribution[dist, zpos, CylRad, CylLen] +
       TopContribution[dist, zpos, CylRad, CylLen] +
       BotContribution[dist, zpos, CylRad, CylLen]
```

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Visualizing the London Potential of a Finite Cylinder

notebook (non-evaluated) pdf (evaluated) html (evaluated)

The example is finished off by visualizing the results. Some of the numerical integrations are still poorly behaved in the vicinity of the cylinder's sharp edge.

1: Demonstrating that the *LondonCylinderPotential* function, that was defined above, gives a numerical result.

2: Here, the potential is visualized with `Plot3D` outside the radius from the mid-plane to above the cylinder.

4: This is perhaps easier to interpret: the r-dependence is plotted at several different midplanes.

6: The same as the above, but for midplanes above the top of the cylinder.

7: `ContourPlot` probably gives the easiest visualization to interpret in this case.

```
1 LondonCylinderPotential[2, .5, 1, 3]

2 Plot3D[LondonCylinderPotential[dist, zpos, 1, 2],
    {dist, 1.1, 3}, {zpos, 0, 3}]

3 << Graphics`Graphics`

  Visualize result as a function of radial distance at different
  altitudes

4 LondonPlot = Plot[
    {LondonCylinderPotential[dist, 0, 1, 4/3],
     LondonCylinderPotential[dist, 2/3, 1, 4/3],
     LondonCylinderPotential[dist, 4/3, 1, 4/3],
     LondonCylinderPotential[dist, 2, 1, 4/3]},
    {dist, 0.01, 3}, PlotStyle →
      {{Thickness[0.02], RGBColor[1, 0, 0]},
       {Thickness[0.015], RGBColor[0, 0.5, 0]},
       {Thickness[0.01], RGBColor[0, 0, 1]},
       {Thickness[0.005], RGBColor[1, 0, 1]}}]

5 Show[LondonPlot, PlotRange → {-5, 3}]

6 TopOfCylinder = Plot[{LondonCylinderPotential[dist, 1.1, 1, 1],
      LondonCylinderPotential[dist, 1.2, 1, 1],
      LondonCylinderPotential[dist, 1.3, 1, 1],
      LondonCylinderPotential[dist, 1.4, 1, 1]}, {dist, 0, 3},
    PlotStyle → {{Thickness[0.02], RGBColor[1, 0, 0]},
      {Thickness[0.015], RGBColor[0, 0.5, 0]},
      {Thickness[0.01], RGBColor[0, 0, 1]},
      {Thickness[0.005], RGBColor[1, 0, 1]}}]

  The contour plot below would take an enormously long
  time to compute if we had not employed all of the ``integral
  tricks''

7 ContourPlot[LondonCylinderPotential[dist, height, 1, 0.25],
    {dist, 0.001, 2}, {height, 0.001, 2},
    Contours -> 25, ColorFunction -> (Hue[0.6 #] &)]
```

Stokes' Theorem

The final generalization of the fundamental theorem of calculus is the relation between a vector function integrated over an oriented surface and another vector function integrated over the closed curve that bounds the surface.

A simplified version of Stokes's theorem has already been discussed—Green's theorem in the plane can be written in full vector form:

$$\begin{aligned}\int\int_R \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y}\right) dxdy &= \int_R \nabla \times \vec{F} \cdot d\vec{A} \\ &= \oint_{\partial R} (F_1 dx + F_2 dy) = \oint_{\partial R} \vec{F} \cdot \frac{d\vec{r}}{ds} ds\end{aligned} \tag{16-6}$$

as long as the region R lies entirely in the $z =$ constant plane.

In fact, Stokes's theorem is the same as the full vector form in Eq. 16-6 with R generalized to an oriented surface embedded in three-dimensional space:

$$\int_R \nabla \times \vec{F} \cdot d\vec{A} = \oint_{\partial R} \vec{F} \cdot \frac{d\vec{r}}{ds} ds \tag{16-7}$$

Plausibility for the theorem can be obtained from Figures 16-14 and 16-15. The curl of the vector field summed over a surface "spills out" from the surface by an amount equal to the vector field itself integrated over the boundary of the surface. In other words, if a vector field can be specified everywhere for a *fixed* surface, then its integral should only depend on some vector function integrated over the boundary of the surface.

Maxwell's equations

The divergence theorem and Stokes's theorem are generalizations of integration that invoke the divergence and curl operations on vectors. A familiar vector field is the electromagnetic field and Maxwell's

equations depend on these vector derivatives as well:

$$\nabla \cdot \vec{B} = 0 \qquad \nabla \times \vec{E} = \frac{\partial \vec{B}}{\partial t}$$
$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{j} \qquad \nabla \cdot \vec{D} = \rho \tag{16-8}$$

in MKS units and the total electric displacement $\vec{D}$ is related to the total polarization $\vec{P}$ and the electric field $\vec{E}$ through:

$$\vec{D} = \vec{P} + \epsilon_o \vec{E} \tag{16-9}$$

where ϵ_o is the dielectric permittivity of vacuum. The total magnetic induction $\vec{B}$ is related to the induced magnetic field $\vec{H}$ and the material magnetization through

$$\vec{B} = \mu_o(\vec{H} + \vec{M}) \tag{16-10}$$

where μ_o is the magnetic permeability of vacuum.

Ampere's Law

Ampere's law that relates the magnetic field lines that surround a static current is a macroscopic version of the (static) Maxwell equation $\nabla \times \vec{H} = \vec{j}$:

Gauss' Law

Gauss' law relates the electric field lines that exit a closed surface to the total charge contained within the volume bounded by the surface. Gauss' law is a macroscopic version of the Maxwell equation $\nabla \cdot \vec{D} = \rho$:

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