Boundary tracing

1. General idea

Given a known solution $T = T(\vec{r})$ to a PDE in two dimensions, we seek boundaries along which the flux condition

$$\boxed{\vec{n} \cdot \vec{\nabla} T = F(\vec{r}, T, \|\vec{\nabla} T\|)} \qquad (1)$$

holds, in an attempt to construct new domains which also admit the same known solution T. Whereas usually the boundary normal $\vec{n}$ is known (given by the shape of the domain) and T is unknown, in boundary tracing, T is known and $\vec{n}$ is unknown: we seek new boundary shapes along which the prescribed flux condition (1) is satisfied.

Geometrically,

$$\boxed{\cos\theta = \frac{F}{\|\vec{\nabla} T\|}}, \qquad (2)$$

where θ is the angle between $\vec{n}$ and $\vec{\nabla} T$. Define the viability function

$$\boxed{\Phi = (\vec{\nabla} T)^2 - F^2}. \qquad (3)$$

- Viable domain: $\|\vec{\nabla} T\| \geq |F|$ or $\Phi \geq 0$

  Traced boundaries exist (there are 2 branches).

- Terminal curve: $\|\vec{\nabla} T\| = |F|$ or $\Phi = 0$

  Traced boundaries terminate.

- Non-viable domain: $\|\vec{\nabla} T\| < |F|$ or $\Phi < 0$

  Traced boundaries do not exist.

In practice, ~~(1) is written in~~ an appropriate coordinate system is chosen for the problem at hand, and (1) is rewritten as an ODE for the sought-after boundary curves, called traced boundaries. From (2) we see that the two traced boundaries through a point are locally symmetric about the T-contour through that point.

2. Theory

A summary of useful results from ML Anderson, AP Bassom & N Fowkes, "Boundary tracing and boundary value problems. I. Theory." Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci (2007) 463, 1909–1924:

2.1 Terminal points

Points along the terminal curve $\|\vec{\nabla} T\| = |F|$ are called terminal points, at which $\cos\theta = \pm 1$ so $\vec{n}$ is parallel to $\vec{\nabla}T$. Thus the traced boundaries through a terminal point are tangential to the local T-contour.

- Ordinary terminal point

  The local T-contour crosses the terminal curve at a non-zero angle. The traced boundaries (which are tangential to the T-contour) terminate in a cusp (they cannot enter the non-viable domain).

- Critical terminal point

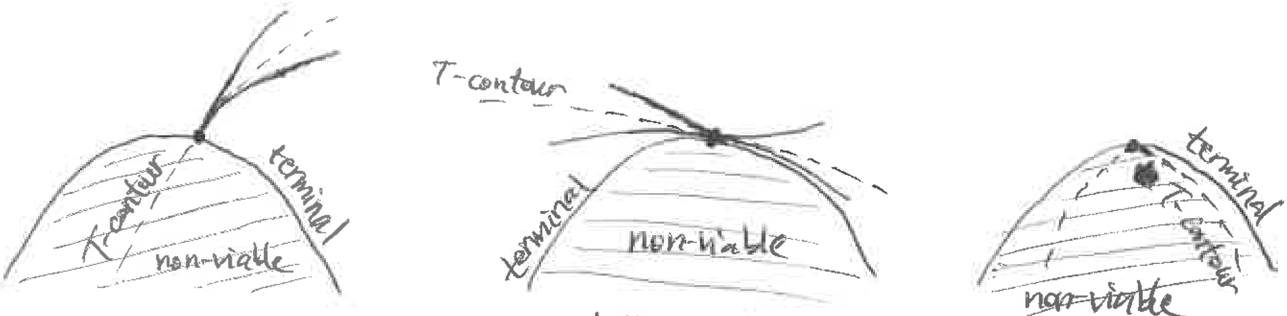
  The local T-contour is tangential to the terminal curve.

  - Hyperbolic case

    The T-contour lies on the viable side of the terminal curve, and there are two smooth traced boundaries which pass through.

  - Elliptic case

    The T-contour lies on the non-viable side of the terminal curve, and there are no smooth traced boundaries which pass through.

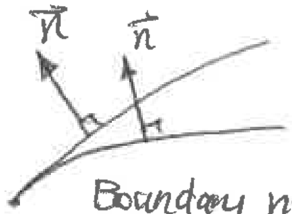


Ordinary terminal point

Hyperbolic critical terminal point

Elliptic critical terminal point

Once the traced boundaries have been determined, the two branches can be patched together almost arbitrarily: the only requirement is that the boundary normal $\vec{n}$ be consistent. At ordinary terminal points the cusp formed is incompatible with this requirement (unless F vanishes or is discontinuous) so domains cannot be constructed using sections of traced boundary which hit ordinary terminal points; thus critical terminal points are very important.



Boundary normals are inconsistent at a cusp

In situations which are highly symmetric, it is also possible to have

- Degenerate case (for a critical terminal point)

  The T-contour coincides ~~■~~ completely with the terminal curve; ~~the~~ all terminal points are critical terminal points. The terminal curve is called a critical terminal curve, and ~~it~~ is itself a traced boundary unto which other traced boundaries attach smoothly.

2.2 Curvature of traced boundaries (see Anderson et al.)

Let $\vec{t}$ be the tangent vector to the boundary, orthogonal to $\vec{n}$. Then the traced boundary curvature is

$$\kappa = \frac{(\vec{n}\cdot\vec{\nabla})(\vec{t}\cdot\vec{\nabla})T - \vec{t}\cdot\vec{\nabla}F}{\vec{t}\cdot\vec{\nabla}T} . \tag{4}$$

Note that the denominator vanishes at terminal points, and if the numerator is non-zero we have $|\kappa| = \infty$ corresponding to the cusps formed at ordinary terminal points.

But if both numerator and denominator of (4) vanish, this corresponds to ~~an ore~~ a critical terminal point, i.e.

$$(\vec{n}\cdot\vec{\nabla})(\vec{t}\cdot\vec{\nabla})T - \vec{t}\cdot\vec{\nabla}F = 0 . \tag{5}$$

After resolving the indeterminate 0/0 in (4), we find that the traced boundary curvature at a critical ~~terminal~~ point is given by the quadratic

$$\kappa^2\left[\vec{n}\cdot\vec{\nabla}T\right] + \kappa\left[2(\vec{t}\cdot\vec{\nabla})^2 T - (\vec{n}\cdot\vec{\nabla})^2 T + \vec{n}\cdot\vec{\nabla}F\right]$$
$$+\left[(\vec{t}\cdot\vec{\nabla})^2 F - (\vec{n}\cdot\vec{\nabla})(\vec{t}\cdot\vec{\nabla})^2 T\right]$$
$$= 0. \tag{6}$$

Additional insight can be gained by mapping traced boundaries onto the boundary tracing manifold

$$z^2 = \Phi(\vec{r}), \tag{7}$$

which crosses the $z = 0$ plane along the terminal curve $\Phi = 0$. In this setting one may derive (see Anderson et al.) results for critical terminal points (hyperbolic and elliptic cases on Page 2) in the manifold and project back to the plane:

- <u>Hyperbolic case</u> ($\kappa_\Phi > \kappa_T$)
  The T-contour lies on the viable side of the terminal curve. The traced boundaries form a saddle in the manifold; the separatrices, when projected back to the plane, form ~~the~~ two smooth traced boundaries.
- <u>Elliptic case</u> ($\kappa_\Phi < \kappa_T$)
  The T-contour lies on the non-viable side of the terminal curve. The traced boundaries form spirals in the manifold, which when projected back to the plane, are ~~not~~ not usable.

(The degenerate case is $\kappa_\Phi = \kappa_T$). Here κ_f is the signed curvature of a contour $f = \text{const}$, given by

$$\kappa_f = \frac{([\times\vec{\nabla}f]\cdot\vec{\nabla})^2 f}{\|\vec{\nabla}f\|^3}, \tag{8}$$

where $\times$ is a 90° rotation operator (the unary, 2D analogue of the usual cross product).

3. Curvilinear coordinates

Here I introduce orthogonal (but otherwise general) curvilinear coordinates in 2D, in preparation for boundary tracing.

Let $\vec{a}_x, \vec{a}_y$ be the standard basis vectors of the usual Cartesian coordinates x, y. Note that $\vec{a}_x$ and $\vec{a}_y$ are universally constant, i.e.

$$\boxed{d\vec{a}_x = d\vec{a}_y = \vec{0}} \; . \tag{9}$$

The position vector is given by

$$\boxed{\vec{r} = x\,\vec{a}_x + y\,\vec{a}_y} \; . \tag{10}$$

Notice how

$$\vec{a}_x = \frac{\partial \vec{r}}{\partial x} \tag{11}$$

$$\vec{a}_y = \frac{\partial \vec{r}}{\partial y} \; . \tag{12}$$

With this in mind, consider the curvilinear coordinates (u, v) given by the transformation

$$x = x(u, v) \tag{13}$$

$$y = y(u, v) \; . \tag{14}$$

A local basis arises from the derivatives of position, in analogy to (11) & (12):

$$\vec{h}_u = \frac{\partial \vec{r}}{\partial u} = \frac{\partial x}{\partial u}\vec{a}_x + \frac{\partial y}{\partial u}\vec{a}_y \tag{15}$$

$$\vec{h}_v = \frac{\partial \vec{r}}{\partial v} = \frac{\partial x}{\partial v}\vec{a}_x + \frac{\partial y}{\partial v}\vec{a}_y \tag{16}$$

We shall assume that our curvilinear coordinate system is orthogonal, i.e.

$$\boxed{\vec{h}_u \cdot \vec{h}_v = 0} \; . \tag{17}$$

Define the scale factors (or Lamé coefficients),

$$\boxed{\begin{aligned} h_u &= \|\vec{h}_u\| \\ h_v &= \|\vec{h}_v\| \end{aligned}} \qquad \begin{aligned}(18)\\(19)\end{aligned}$$

Normalising $\vec{h}_u$ and $\vec{h}_v$, we obtain the local orthonormal basis,

$$\boxed{\begin{aligned} \vec{a}_u &= \frac{\vec{h}_u}{h_u} \\ \vec{a}_v &= \frac{\vec{h}_v}{h_v} \end{aligned}} \; . \qquad \begin{aligned}(20)\\(21)\end{aligned}$$

We shall assume that this basis is right-handed, i.e.

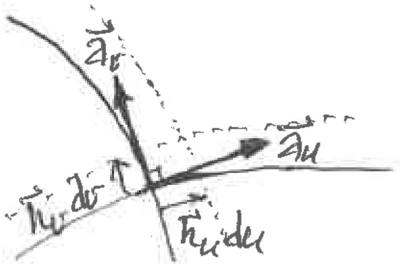
$$\boxed{\vec{a}_v = \times \vec{a}_u} \; , \qquad (22)$$

where $\times$ is the 2D (unary) analogue of the cross product, and rotates a vector 90° anti-clockwise.

3.1 Differential displacement

Incrementing u by du whilst keeping v fixed, results in the infinitesimal displacement $\vec{h}_u du$; incrementing v by dv whilst keeping u fixed, results in the infinitesimal displacement $\vec{h}_v dv$. In symbols:

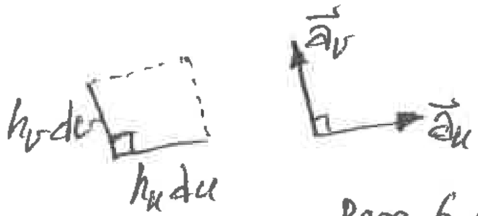
$$\begin{aligned} d\vec{r} &= \frac{\partial \vec{r}}{\partial u} du + \frac{\partial \vec{r}}{\partial v} dv \\ &= \vec{h}_u du + \vec{h}_v dv \end{aligned}$$



$$\boxed{d\vec{r} = h_u du\, \vec{a}_u + h_v dv\, \vec{a}_v} \; . \qquad (23)$$

The four contours (two for u and two for v) form an infinitesimal rectangle aligned with the local orthonormal basis, with sides of length $h_u du$ and $h_v dv$. Thus the infinitesimal area element is

$$\boxed{dV = h_u h_v \, du\, dv} \; . \qquad (24)$$



3.2 Gradient

Consider a scalar field T. Observe that

$$dT = \frac{\partial T}{\partial u}\,du + \frac{\partial T}{\partial v}\,dv$$
$$= \left(\frac{1}{h_u}\frac{\partial T}{\partial u}\right)(h_u\,du) + \left(\frac{1}{h_v}\frac{\partial T}{\partial v}\right)(h_v\,dv). \qquad (25)$$

Now by definition of the gradient, we also have

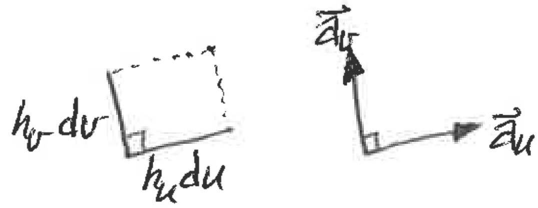
$$dT = \vec{\nabla} T \cdot d\vec{r}$$
$$= \vec{\nabla} T \cdot (h_u\,du\,\vec{a}_u + h_v\,dv\,\vec{a}_v) \qquad (26)$$

where we have used (23). Comparing (25) and (26), we see that

$$\boxed{\vec{\nabla} T = \frac{1}{h_u}\frac{\partial T}{\partial u}\vec{a}_u + \frac{1}{h_v}\frac{\partial T}{\partial v}\vec{a}_v}\;. \qquad (27)$$

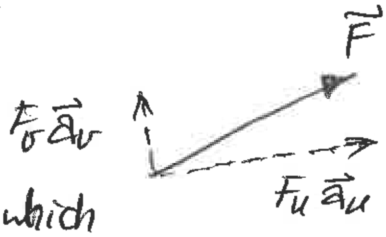
3.3 Divergence

Consider a vector field $\vec{F} = F_u\vec{a}_u + F_v\vec{a}_v$, and the infinitesimal rectangle formed by effecting the increments du and dv.



The net flux across the two edges normal to $\vec{a}_u$, which have length $h_v\,dv$, is

$$\frac{\partial}{\partial u}(F_u \cdot h_v\,dv)\cdot du.$$



The net flux across the two edges normal to $\vec{a}_v$, which have length $h_u\,du$, is

$$\frac{\partial}{\partial v}(F_v \cdot h_u\,du)\cdot dv\;.$$

Summing these we obtain the total flux across the rectangle, which, divided by its area, the area element (24), yields the divergence

$$\boxed{\vec{\nabla}\cdot\vec{F} = \frac{1}{h_u h_v}\left[\frac{\partial}{\partial u}(h_v F_u) + \frac{\partial}{\partial v}(h_u F_v)\right]}\;. \qquad (28)$$

4. Boundary tracing in curvilinear coordinates

Here I derive the boundary tracing ODEs for orthogonal (but otherwise general) curvilinear coordinates under various parametrisations.

4.1 Boundary normal

The tangent vector to any curve is the ~~normalised~~ unit vector of the differential displacement (23),

$$\boxed{\vec{t} = \frac{h_u\,du\,\vec{a}_u + h_v\,dv\,\vec{a}_v}{ds}} \qquad (29)$$

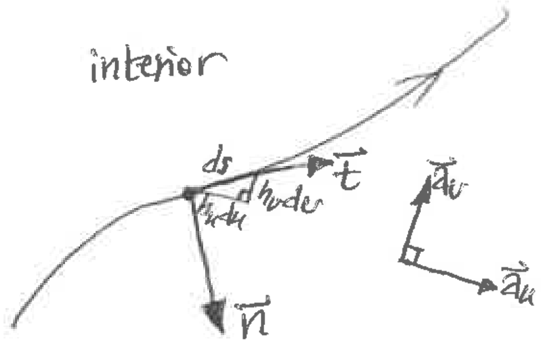
where ds is the differential arc length

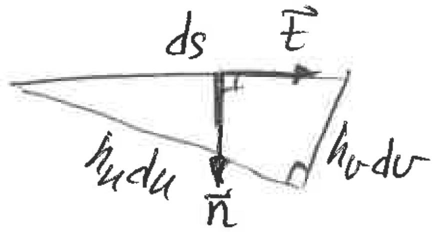
$$\boxed{ds = \|d\vec{r}\| = \sqrt{(h_u\,du)^2 + (h_v\,dv)^2}} \qquad (30)$$

Identifying the interior to the left of the direction of travel, the outward boundary normal is

$$\vec{n} = -[\times\vec{t}]$$

$$\boxed{\vec{n} = \frac{h_v\,dv\,\vec{a}_u - h_u\,du\,\vec{a}_v}{ds}} \qquad (31)$$





4.2 Abbreviations

For brevity define

$$\boxed{\begin{aligned} d\mu &= h_u\, du \\ d\upsilon &= h_v\, dv \\ P &= \frac{1}{h_u}\frac{\partial T}{\partial u} \\ Q &= \frac{1}{h_v}\frac{\partial T}{\partial v} \end{aligned}}$$

(32)
(33)
(34)
(35)

and

$$\boxed{\begin{aligned} \alpha &= \frac{d\mu}{ds} \\ \beta &= \frac{d\upsilon}{ds} \end{aligned}}$$

(36)
(37)

Then

$$\boxed{\begin{aligned} d\vec{r} &= d\mu\, \vec{a}_u + d\upsilon\, \vec{a}_v \\ \vec{\nabla} T &= P\, \vec{a}_u + Q\, \vec{a}_v \\ \vec{n} &= \frac{d\upsilon\, \vec{a}_u - d\mu\, \vec{a}_v}{ds} \\ &= \beta\, \vec{a}_u - \alpha\, \vec{a}_v \\ ds &= \sqrt{d\mu^2 + d\upsilon^2} \end{aligned}}$$

(38)
(39)
(40)
(41)
(42)

Note that

$$P^2 + Q^2 = (\vec{\nabla} T)^2 \quad (43)$$

$$\alpha^2 + \beta^2 = 1 \,. \quad (44)$$

4.3 Coordinate parametrisation

For traced boundaries parametrised as $v = v(u)$, we use (40), (42) and (39) so that the flux condition (1) becomes

$$\frac{dv\,\vec{a}_u - du\,\vec{a}_v}{\sqrt{du^2+dv^2}} \cdot (P\vec{a}_u + Q\vec{a}_v) = F$$

$$(P\,dv - Q\,du)^2 = F^2(du^2+dv^2),$$

yielding the quadratic

$$(P^2-F^2)\,dv^2 - 2PQ\,dv\,du + (Q^2-F^2)\,du^2 = 0. \tag{45}$$

The discriminant, quartered, is

$$\begin{aligned}
&(PQ)^2 - (P^2-F^2)(Q^2-F^2) \\
&= \cancel{P^2Q^2} - [\cancel{P^2Q^2} - (P^2+Q^2)F^2 + F^4] \\
&= (P^2+Q^2)F^2 - F^4 \\
&= (\nabla T)^2 F^2 - F^4 \\
&= F^2[(\nabla T)^2 - F^2] \\
&= F^2\Phi;
\end{aligned}$$

therefore the tracing ODE is

$$\boxed{\frac{dv}{du} = \frac{PQ \pm F\sqrt{\Phi}}{P^2-F^2}}. \tag{46}$$

Alternatively, for the parametrisation $u = u(v)$,

$$\boxed{\frac{du}{dv} = \frac{PQ \mp F\sqrt{\Phi}}{Q^2-F^2}}. \tag{47}$$

In particular, for Cartesian coordinates (x, y), (46) reduces to

$$\frac{dy}{dx} = \frac{\frac{\partial T}{\partial x}\frac{\partial T}{\partial y} \pm F\sqrt{\Phi}}{\left(\frac{\partial T}{\partial x}\right)^2 - F^2}.$$

4.4 Arc length parametrisation

The coordinate ~~trans~~ parametrisations $u=u(v)$ and $v=v(u)$ will, in numerical contexts, be problematic if du/dv or dv/du ever become infinite. To avoid this, we may use the arc length parametrisation $u=u(s)$, $v=v(s)$. Using (41) and (39), the flux condition (1) becomes

$$(\beta\vec{a}_u-\alpha\vec{a}_v)\cdot(P\vec{a}_u+Q\vec{a}_v)=F,$$

which, with (44), comprise the system

$$\boxed{\begin{aligned}P\beta-Q\alpha&=F\\ \alpha^2+\beta^2&=1\end{aligned}}\,. \qquad \begin{aligned}&(45)\\&(46)\end{aligned}$$

From (45),

$$P\beta=F+Q\alpha$$
$$P^2\beta^2=F^2+2FQ\alpha+Q^2\alpha^2.$$

Using (46), this becomes

$$P^2(1-\alpha^2)=F^2+2FQ\alpha+Q^2\alpha^2,$$

yielding the quadratic

$$(P^2+Q^2)\alpha^2+2FQ\alpha+(F^2-P^2)=0. \qquad (47)$$

The discriminant, quartered, is

$$\begin{aligned}&(FQ)^2-(P^2+Q^2)(F^2-P^2)\\ &=\cancel{F^2Q^2}-[P^2F^2+\cancel{Q^2F^2}-(P^2+Q^2)P^2]\\ &=-P^2F^2+(P^2+Q^2)P^2\\ &=-P^2F^2+(\vec{\nabla}T)^2P^2\\ &=P^2[(\vec{\nabla}T)^2-F^2]\\ &=P^2\Phi.\end{aligned}$$

Therefore

$$\alpha=\frac{-FQ\pm P\sqrt{\Phi}}{P^2+Q^2}=\frac{-QF\pm P\sqrt{\Phi}}{(\vec{\nabla}T)^2},$$

and $\beta = \frac{1}{P}(F + Q\alpha)$

$$= \frac{1}{P}\left(\frac{(P^2+Q^2)F}{(\vec{\nabla}T)^2} + \frac{-Q^2F \pm PQ\sqrt{\Phi}}{(\vec{\nabla}T)^2}\right)$$

$$= \frac{P^2F \pm PQ\sqrt{\Phi}}{P(\vec{\nabla}T)^2} .$$

Thus the tracing system of ODEs under arc length parametrisation is

$$\boxed{\begin{aligned} \frac{du}{ds} &= \alpha = \frac{-QF \pm P\sqrt{\Phi}}{(\vec{\nabla}T)^2} \qquad (48) \\ \frac{dv}{ds} &= \beta = \frac{PF \pm Q\sqrt{\Phi}}{(\vec{\nabla}T)^2} \qquad (49) \end{aligned}} .$$

4.5 Arc length parametisation ~~for~~ for contours

Consider the similar problem of parametrising a contour, $T = \text{const}$, by arc length. By definition this is given by $dT = \vec{\nabla}T \cdot d\vec{r} = 0$. Thus, using (37) and (38), we have

$$P\,du + Q\,dv = 0 ,$$

or

$$\boxed{P\alpha + Q\beta = 0} \qquad (50)$$

in the place of (45). This amounts to applying the replacements $\{P \to Q, Q \to -P, F \to 0\}$ to (45), which leaves $(\vec{\nabla}T)^2$ invariant. Applying these same replacements unto (48) & (49), we obtain the contour system of ODEs

$$\boxed{\begin{aligned} \frac{du}{ds} &= \alpha = \frac{\pm Q}{\|\vec{\nabla}T\|} \qquad (51) \\ \frac{dv}{ds} &= \beta = \frac{\mp P}{\|\vec{\nabla}T\|} \qquad (52) \end{aligned}} ,$$

where we have used $\sqrt{\Phi} = \sqrt{(\vec{\nabla}T)^2 - F^2} \to \|\vec{\nabla}T\|$.

4.6 Summary

With $P = \frac{1}{h_u}\frac{\partial T}{\partial u}$ and $Q = \frac{1}{h_v}\frac{\partial T}{\partial v}$, we have the following:

4.6.1 Traced boundary $v = v(u)$

$$\boxed{\frac{dv}{du} = \frac{h_u}{h_v} \cdot \frac{PQ \pm F\sqrt{\Phi}}{P^2 - F^2}} \tag{53}$$

4.6.2 Traced boundary $u = u(v)$

$$\boxed{\frac{du}{dv} = \frac{h_v}{h_u} \cdot \frac{PQ \mp F\sqrt{\Phi}}{Q^2 - F^2}} \tag{54}$$

4.6.3 Traced boundary $u = u(s)$, $v = v(s)$

$$\frac{du}{ds} = \frac{-QF \pm P\sqrt{\Phi}}{h_u (\vec{\nabla} T)^2} \tag{55}$$

$$\frac{dv}{ds} = \frac{PF \pm Q\sqrt{\Phi}}{h_v (\vec{\nabla} T)^2} \tag{56}$$

4.6.4 T-contour $u = u(s)$, $v = v(s)$

$$\frac{du}{ds} = \frac{\pm Q}{h_u \|\vec{\nabla} T\|} \tag{57}$$

$$\frac{dv}{ds} = \frac{\mp P}{h_v \|\vec{\nabla} T\|} \tag{58}$$