PDE COURSE

VERY SHORT INTRO TO DIFFUSION

WE ASSUME $\boxed{u(t,\vec{x})}$ GIVES THE DENSITY OF (---) AS A FUNCTION OF TIME AND POINT $\boxed{\vec{x}}$

WE ASSUME $\boxed{\frac{\partial u}{\partial t}(t,\vec{x}_0)}$, VARIATION OF $\boxed{u}$ IN TIME KEEPING $\vec{x}_0$ FIXED, DEPENDS ON THE DIFFERENCE BETWEEN $u(t,\vec{x}_0)$ AND THE AVERAGE ON A SMALL VOLUME CENTERED IN $\vec{x}_0$ OF u, $\bar{u}$

$$\frac{\partial u(t,\vec{x}_0)}{\partial t} \propto -u+\bar{u}$$

$\bar{u}$ COMPUTED ON $V\to 0$ (LOCAL PROPERTY)

WE CHOOSE THE SIGN IN A WAY THAT IF THE AVERAGE AROUND THE POINT IS HIGHER THAN IN THE POINT, $\frac{\partial u}{\partial t}>0$, THE DENSITY GROWS, OTHERWISE ...

u GOES WHERE THERE IS LESS, DIFFUSES. IT IS EASY TO SEE THAT IF $u(0,\vec{x})\geq 0$ $\forall \vec{x} \Rightarrow u(t,\vec{x})\geq 0$ $\forall \vec{x}, t>0$, SINCE A POINT WITH $u\geq 0$ MAY BECOME NEGATIVE ONLY IF IT HAS NEGATIVE POINTS AROUND.

WE WOULD LIKE TO EXPRESS $\lim_{V\to 0}(\bar{u}-u)$ USING PARTIAL DERIVATIVE, TO OBTAIN A PDE

THE GEOMETRICAL (AND PHYSICAL) MEANING OF VECTOR CALCULUS AND CURVILINEAR COORDINATES

LET US CONSIDER TWO POINTS, A, B, REPRESENTED IN CART. COORD. AS

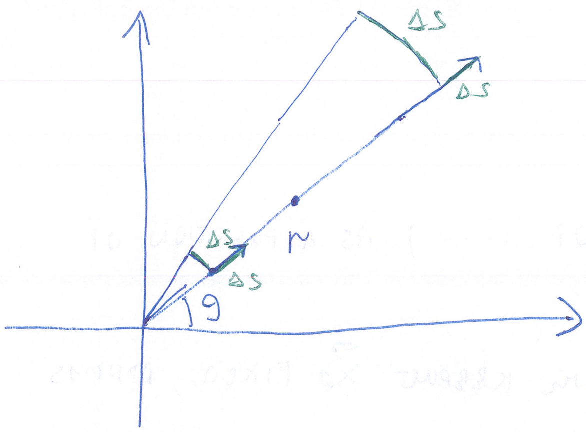
$A(x,y)$ $\quad$ $B(x+\Delta x, y+\Delta y)$

WE KNOW THAT THEIR DISTANCE IS GIVEN BY

$$\Delta s^2 = \Delta x^2 + \Delta y^2$$

WE MAY WRITE THIS AS $ds^2 = dx^2 + dy^2$, MEANING THAT dx, dy ARE SMALL, AND WE WILL RETAIN ONLY THE LOWEST TERMS IN THE FOLLOWING

FIG 1



WE MAY USE OTHER COORDINATES IN THE PLANE

$$r, \theta$$

$$x = r\cos\theta \qquad y = r\sin\theta$$

IF WE SEE x AS A FUNCTION OF $x(r,\theta)$ WE MAY USE TAYLOR EXPANSION TO WRITE

$$\Delta x = \frac{\partial x}{\partial \theta}\Delta\theta + \frac{\partial x}{\partial r}\Delta r + (\text{higher order})$$

AS STATED ABOVE, WE ASSUME THE Δ SMALL $(\Delta \to 0)$ AND KEEP ONLY THE FIRST ORDER. TO REMAND THIS, WE WRITE

$$dx = \frac{\partial x}{\partial \theta} d\theta + \frac{\partial x}{\partial r} dr$$

FROM

$$\frac{dx}{dr} = \cos\theta \qquad \frac{dx}{d\theta} = -r\sin\theta \qquad \frac{dy}{dr} = \sin\theta \qquad \frac{dy}{d\theta} = r\cos\theta$$

WE GET

$$ds^2 = r^2 d\theta^2 + dr^2$$

THE CONTRIBUTION OF $d\theta$ TO ds IS WEIGHTED BY A FACTOR r AS GROW. CLEAR ALSO FROM FIG. 1

THIS WILL HAPPEN IN GENERAL WITH CURV. COORD.

$$X(q_1,q_2,q_3) \quad Y(q_1,q_2,q_3) \quad Z(q_1,q_2,q_3) \quad \text{OR} \quad x_i(q_i)$$

$$ds^2 = \sum_i dx_i dx_i = \sum_{i,j,n}\left(\frac{\partial x_i}{\partial q_j} dq_j\right)\left(\frac{\partial x_i}{\partial q_n} dq_n\right) =$$

$$= \sum_{j,n}\left(\sum_i \frac{\partial x_i}{\partial q_j}\frac{\partial x_i}{\partial q_n}\right) dq_j dq_n$$

WE ARE INTERESTED ONLY IN ORTHOGONAL COORDINATES, FOR WHICH

$$ds^2 = h_1^2(q_1,q_2,q_3)\, dq_1^2 + h_2^2(q_1,q_2,q_3)\, dq_2^2 + h_3^2(q_1,q_2,q_3)\, dq_3^2$$

FOR EXAMPLE, SPHERICAL

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta \, d\varphi^2$$

$h_1 = 1$
$h_2 = r$
$h_3 = r \sin\theta$

OR CYLINDRICAL (FROM WHICH WE GET 2D POLAR $dz = 0$)

$$ds^2 = dr^2 + r^2 d\theta^2 + dz^2$$

$h_1 = 1$
$h_2 = r$
$h_3 = 1$

THE GRADIENT

$\vec{\nabla}\phi$ IS GEOMETRICALLY DEFINED IN SUCH A WAY THAT, IF A AND B ARE SEPARATED BY $\vec{\Delta S} = B - A$, $\vec{\nabla}\phi \cdot \vec{\Delta S}$ GIVES (FIRST ORDER) $\phi(B) - \phi(A) \equiv \Delta\phi$

IN CARTESIAN COORDINATES (2D)

$$(\vec{\nabla}\phi)_x (\vec{\Delta S})_x + (\vec{\nabla}\phi)_y (\vec{\Delta S})_y = (\vec{\nabla}\phi)_x \Delta x + (\vec{\nabla}\phi)_y \Delta y = \Delta\phi$$

BUT WE ALSO HAVE

$$\Delta\phi = \frac{\partial\phi}{\partial x}\Delta x + \frac{\partial\phi}{\partial y}\Delta y \Rightarrow \boxed{(\nabla\phi)_i = \frac{\partial\phi}{\partial x_i}}$$

(WE MAY WRITE AGAIN $d\phi = \frac{\partial\phi}{\partial x}dx + \frac{\partial\phi}{\partial y}dy$ TO RECALL THAT WE WANT FIRST ORDER)

THIS IS NOT TRUE IN CURV. COORD., IF WE WANT TO KEEP THE GEOMETRICAL MEANING OF THE GRADIENT

$B - A = \vec{\Delta S}$ HAS THE SAME MEANING OF COORDINATES

$$(\vec{\Delta S})_r = \Delta r \qquad \text{BUT} \qquad (\vec{\Delta S})_\theta = r\,\Delta\theta$$

ALONG THE (VARYING) VECTOR $\vec{e}_\theta$ ATTACHED IN r

$$\Rightarrow (\vec{\nabla}\phi)\cdot(\vec{\Delta S}) = (\vec{\nabla}\phi)_r \Delta r + (\vec{\nabla}\phi)_\theta \, r\Delta\theta$$

$$\underset{\parallel}{\Delta\phi} = \frac{\partial\phi}{\partial r}\Delta r + \frac{\partial\phi}{\partial\theta}\Delta\theta \Rightarrow \boxed{(\nabla\phi)_r = \frac{\partial\phi}{\partial r} \qquad (\nabla\phi)_\theta = \frac{1}{r}\frac{\partial\phi}{\partial\theta}}$$

IN GENERAL

$$\sum_i \frac{\partial\phi}{\partial q_i}\Delta q_i = \Delta\phi = \sum_i h_i(\vec q)\,\Delta q_i\,(\vec\nabla\phi)_i$$

$$\Rightarrow \quad (\vec\nabla\phi)_i = \frac{\partial\phi}{\partial q_i}\,\frac{1}{h_i(\vec q)}$$

EXAMPLES:

$$(\vec\nabla\phi)_r = \frac{\partial\phi}{\partial r} \qquad (\vec\nabla\phi)_\theta = \frac{1}{r}\frac{\partial\phi}{\partial\theta} \qquad (\vec\nabla\phi)_\varphi = \frac{1}{r\sin\theta}\frac{\partial\phi}{\partial\varphi}$$

$$(\vec\nabla\phi)_r = \frac{\partial\phi}{\partial r} \qquad (\vec\nabla\phi)_\theta = \frac{1}{r}\frac{\partial\phi}{\partial\theta} \qquad (\vec\nabla\phi)_z = \frac{\partial\phi}{\partial z}$$

THE DIVERGENCE

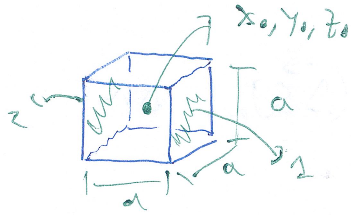
LET US CONSIDER THE VECTOR FIELD $\vec A(\vec x)$

WE DEFINE $\mathrm{div}(\vec A)$ OR $\vec\nabla\cdot\vec A$ AS

$$\mathrm{div}(\vec A)_{\vec x} = \lim_{V\to 0}\frac{1}{V}\int_S \vec A\cdot\vec n\, ds$$

REMEMBERING THE DEF. OF 3D RIEMANN INTEGRAL, WE OPERATE ON A SMALL CUBE CENTRED IN x_0, y_0, z_0 AND OF SIZE

$$\Delta x = \Delta y = \Delta z = a \to 0$$



LET US FIRST COMPUTE THE CONTRIBUTION ON THE SIDE 1, THAT WE MAY CALL

$$I_1 = \int_{-\frac{a}{2}}^{\frac{a}{2}} dz \int_{-\frac{a}{2}}^{\frac{a}{2}} dy\; A_x\left(x_0+\frac{\Delta x}{2},\, y_0+y,\, z_0+z\right)$$

WE USE

$$A_x\left(x_0+\frac{\Delta x}{2}, y_0+y, z_0+z\right) = A\left(x_0+\frac{\Delta x}{2}, y_0, z_0\right) +$$

$$+ \frac{\partial A_x}{\partial y}(x_0, y_0, z_0)\, y + \frac{\partial A_x}{\partial z}(x_0, y_0, z_0)\, z + O(y^2, z^2)$$

WHEN INTEGRATING, THE LINEAR TERMS ARE EQUAL TO 0, WHILE THE QUADRATIC TERMS WILL GIVE A a^4 CONTRIBUTION, GOING TO ZERO WITH DIVIDED BY THE VOLUME $\frac{a^4}{a^3} \to 0$

FOR SIMPLICITY WE USE $\Delta x = \Delta y = \Delta z = a$, BUT IS USEFUL TO LEAVE THE DIFFERENCES

$$\Rightarrow \quad I_1 \simeq A_x\left(x_0+\frac{\Delta x}{2}, y_0, z_0\right) \Delta y \Delta z$$

$$\Rightarrow \quad I_1 + I_2 = \left[A_x\left(x_0+\frac{\Delta x}{2}, y_0, z_0\right) - \left(A_x - \frac{\Delta x}{2}, y_0, z_0\right)\right] \Delta y \Delta z$$

$$= \left.\frac{\partial A_x}{\partial x}\right|_{(x_0, y_0, z_0)} \Delta x \Delta y \Delta z$$

DOING THE SAME FOR ALL SIDES

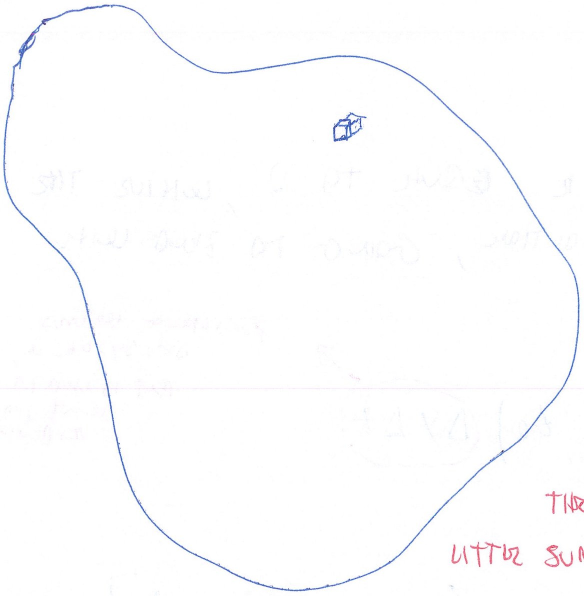
$$\Rightarrow \quad \mathrm{div}(\vec{A}) = \frac{1}{\cancel{\Delta x \Delta y \Delta z}} \left[\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial x}\right] \cancel{\Delta x \Delta y \Delta z}$$

$$\Rightarrow \quad \mathrm{div}(\vec{A}) = \sum_i \frac{\partial A_i}{\partial x_i}$$

AGAIN, IF WE WANT TO PRESERVE THE GEOMETRICAL MEANING, THE FORMULA WILL BE DIFFERENT FOR CURV. COORD.

BEFORE DOING THAT, WE MAY JUSTIFY GAUSS THEOREM

WE USE ANOTHER INTEGRAL APPROACH



$$\int_V \mathrm{div}(\vec{A}) = \sum_i \int_{V_i} \mathrm{div}(\vec{A}) =$$

$$= \sum_i \int_{S_i} \vec{A}\cdot\vec{n} = \int_S \vec{A}\cdot\vec{n}$$

THERE IS A DIFFERENCE BETWEEN SUMMING ALL THE LITTLE SURFACES AND THE OVERALL SURFACE,

BUT CONTRIBUTIONS ON INNER CUBES CANCEL EACH OTHER!

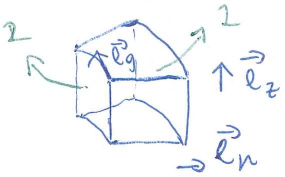
— o —

LET US THINK ABOUT THE CURV. CASE

WE USE AS AN EXAMPLE CILINDRICAL

$$\vec{A} = A_r \vec{e}_r + A_\theta \vec{e}_\theta + A_z \vec{e}_z$$

$\vec{e}_\theta, \vec{e}_z, \vec{e}_r$ LOCALLY DEFINED ORTHONORMAL VECTOR



LET US FIRST COMPUTE THE CONTRIBUTION $I_1 + I_2$

WE ARE WORKING ON $r =$ CONST SURFACES

ALL CONSIDERATIONS INVOLVING TAYLOR EXP. ARE UNCHANGED, SINCE

$$\boxed{\frac{\partial f}{\partial q}\Delta q \simeq \Delta f}$$

IS VALID ALSO FOR CURV. COORD.

BUT CONSIDERATIONS REGARDING INTEGRALS (SURFACE, VOLUME) ARE CHANGED!

→ AREA CONTRIBUTION OF θ !

$$I_1 + I_2 \simeq A_r\left(r_0 + \frac{\Delta r}{2}, \theta_0, z_0\right)\left(\overline{\left[r_0 + \frac{\Delta r}{2}\right]\Delta\theta}\right)\Delta z$$

$$- A_r\left(r_0 + \frac{\Delta r}{2}, \theta_0, z_0\right)\left(\left[r_0 - \frac{\Delta r}{2}\right]\Delta\theta\right)\Delta t$$

$$\Rightarrow \frac{I_1 + I_2}{V} \simeq \frac{1}{\cancel{\Delta r \Delta z (r_0 \Delta\theta)}} \frac{\partial}{\partial r}\left[A_r(r_0, \theta_0, z_0)\, r\right] \cancel{\Delta\theta \Delta z \Delta r}$$

WE WROTE IT IN SUCH A WAY THAT WE MAY EASILY GENERALISE

$$\Rightarrow \mathrm{div}(\vec{A}) = \frac{1}{\underbrace{h_1(\vec{q})h_2(\vec{q})h_3(\vec{q})}_{\text{VOLUME}}}\left[\frac{\partial}{\partial q_1}\left[\overbrace{A_1(\vec{q})h_2(\vec{q})h_3(\vec{q})}^{\text{SURFACE AT } q_1 \text{ CONST}}\right] + \frac{\partial}{\partial q_2}\left[A_2 h_1 h_3\right] + \frac{\partial}{\partial q_3}\left[A_3 h_1 h_2\right]\right]$$

EXAMPLES (POLAR = CILINDRICAL WITH $dz = 0$)

S.C.

$$\frac{1}{r^2 \sin\theta}\left[\frac{\partial}{\partial r}\left(r^2 \sin\theta\, A_r\right) + \frac{\partial}{\partial \theta}\left(r \sin\theta\, A_\theta\right) + \frac{\partial}{\partial \varphi}\left[r A_\varphi\right]\right]$$

CIL

$$\frac{1}{r}\left[\frac{\partial}{\partial r}\left(r A_r\right) + \frac{\partial}{\partial \theta}\left(A_\theta\right) + \frac{\partial}{\partial z}\left(r A_z\right)\right]$$

⇒

$$\mathrm{div}(\vec{A}) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 A_r\right) + \frac{1}{r \sin\theta}\frac{\partial}{\partial\theta}\left(A_\theta \sin\theta\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\left(A_\varphi\right)$$

$$\mathrm{div}(\vec{A}) = \frac{1}{r}\frac{\partial}{\partial r}\left(r A_r\right) + \frac{1}{r}\frac{\partial}{\partial\theta} A_\theta + \frac{\partial}{\partial r}\left(A_z\right)$$

⇒ N.B. THE DIMENSIONALITY OF $\mathrm{div}(\vec{A})$ IS $\frac{[A]}{[L]}$!!

LAPLACIAN

IN CART. COORD.

$$\mathrm{div}(\vec{\nabla}\phi) \equiv \nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial x^2}$$

BUT IN CURV. COORD.

$$(\vec{\nabla}\phi)_i = \frac{1}{h_i(\vec{q})}\frac{\partial\phi}{\partial q_i}$$

$\Rightarrow$

$$\nabla^2\phi = \mathrm{div}(\vec{\nabla}\phi) =$$

$$= \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left[h_2 h_3 \frac{1}{h_1}\frac{\partial\phi}{\partial q_1}\right] + \frac{\partial}{\partial q_2}\left[h_1 h_3 \frac{1}{h_2}\frac{\partial\phi}{\partial q_2}\right] + \frac{\partial}{\partial q_3}\left[h_1 h_2 \frac{1}{h_3}\frac{\partial\phi}{\partial q_3}\right]\right]$$

BY SUBSTITUTION AND TAKING OUT FROM DERIVATIVE IF POSSIBLE WE GET

S.C.

$$\nabla^2\phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\phi}{\partial\varphi^2}$$

C.C.

$$\nabla^2\phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2} + \frac{\partial^2\phi}{\partial z^2}$$

$$[\nabla^2\phi] = \frac{[\phi]}{[L^2]}$$

BUT, WHAT IS THE GEOMETRICAL MEANING OF

$\nabla^2 \phi$?

AT THE BEGINNING, WE WROTE A DIFFUSION EQ. AS

$$\frac{\partial u}{\partial t} \propto \lim_{V \to 0} \left(\bar{u} - u \right)$$

ORDER a

LET US COMPUTE $\bar{\phi}$ ON A SMALL CUBE CENTRED IN (x_0, y_0, z_0)

$$\phi(x,y,z) = \phi(x_0, y_0, z_0) + \frac{\partial \phi}{\partial x}(x - x_0) + \frac{\partial \phi}{\partial y}(y - y_0) + \frac{\partial \phi}{\partial z}(z - z_0) +$$

$$+ \frac{\partial \phi}{\partial x \partial y}(x - x_0)(y - y_0) + \cdots + \frac{1}{2}\frac{\partial \phi}{\partial x^2}(x - x_0)^2 + \quad + \text{ cubic terms}$$

$$\bar{\phi} = \frac{1}{a^3} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx \int_{-\frac{a}{2}}^{\frac{a}{2}} dy \int_{-\frac{a}{2}}^{\frac{a}{2}} dz \; \phi(x,y,z)$$

THESE GO TO 0 WHEN INTEGR. IN $\int_{-\frac{a}{2}}^{\frac{a}{2}}$

$$= \phi(x_0, y_0, z_0) + \frac{1}{a^3} \left(\iiint \text{linear terms} + \iiint \Delta x \Delta y + \Delta x \Delta z + \Delta y \Delta z \right.$$

$$\left. + \frac{1}{2} \iiint \frac{\partial^2 \phi}{\partial x^2} \Delta x^2 + \frac{\partial^2 \phi}{\partial y^2} \Delta y^2 + \frac{\partial^2 \phi}{\partial z^2} \Delta z^2 \right)$$

EACH INTEGRAL CONTRIBUTES AS

$$\frac{a^2}{2} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx \frac{\partial \phi}{\partial x^2}(x_0, y_0, z_0)\, x^2 + \cdots$$

$$= \frac{a^2}{2} \frac{\partial \phi}{\partial x^2} \left[\frac{x^3}{3} \right]_{-\frac{a}{2}}^{a/2} = \frac{a^5}{6} \left[\frac{2}{8} \right] = \frac{a^5}{24}$$

$$\Rightarrow \quad \bar{\phi} - \phi = \frac{a^2}{24} \left(\nabla^2 \phi \right)$$

THE GEOMETRICAL MEANING OF $\nabla^2 \phi$ (COORDINATE INDEPENDENT) IS THAT OF THE LEADING ORDER IN THE CHANGE BETWEEN $\bar{\phi}$ AND ϕ

FOR THIS REASON WE CALL

$$\boxed{\frac{\partial u(t,\vec{x})}{\partial t} = k \nabla^2 u(t,\vec{x})}$$

A DIFFUSION EQUATION