# Conservation Laws

Let $u(\vec{x}, t)$ be the concentration of something at position $\vec{x} \in \Omega$ and time $t$. For instance

$$u = \text{mass density of a fluid (gas)}$$

$$u = \text{chemical concentration}$$

$$u = \text{population density of an organism}$$

$$u = \text{ionic concentration}$$

Then at any given instant
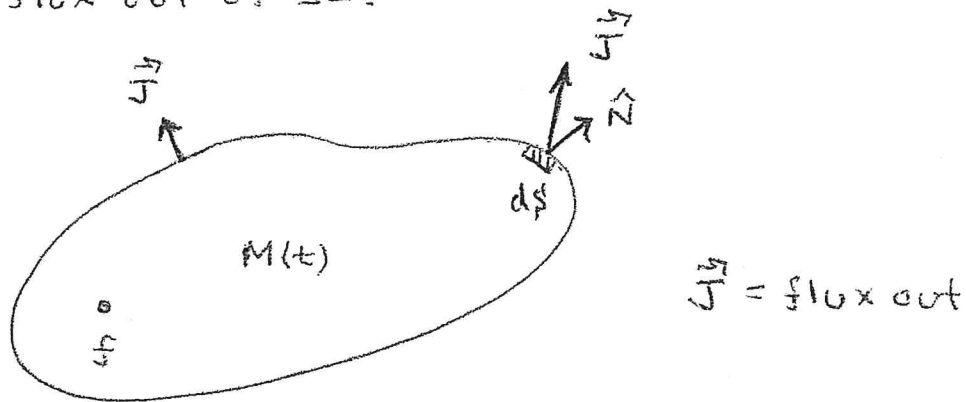
$$M(t) = \int_\Omega u(\vec{x}, t)\, d\vec{x}$$

is the total amount at time $t$. Here $M$ could be total mass, population or net charge

Let

$$\vec{J} = \text{flux of } u \text{ at } \vec{x} \in \Omega$$

$$f = \text{internal sources or sinks of } u \text{ at } \vec{x}. \text{ For instance if } u \text{ is a chemical concentration } f(\vec{x}, t, u) \text{ is the local production rate per unit volume}$$

If $u$ is conserved the rate of change of $M$ must balance the rate of production and flux out of $\Omega$.



$\vec{J}$ = flux out

For <u>any domain</u> $\Omega$

$$\frac{d}{dt} \int_\Omega u(\vec{x}, t)\, d\vec{x} = -\int_{\partial\Omega} \vec{J} \cdot \hat{N}\, ds + \int_\Omega f(\vec{x}, t, u)\, d\vec{x}$$

where the minus sign indicates a flux out.

Assuming $u$ is sufficiently smooth and applying the Divergence theorem

$$\int_\Omega \frac{\partial u}{\partial t}\, d\vec{x} = -\int_\Omega \vec{\nabla} \cdot \vec{J}\, d\vec{x} + \int_\Omega f(\vec{x}, t, u)\, d\vec{x}$$

If the integrands are continuous then since the <u>domain is arbitrary</u> the integrands on each side must match:

(i)
$$\frac{\partial u}{\partial t} = -\vec{\nabla} \cdot \vec{J} + f(\vec{x}, t, u)$$

Differential form of conservation law.

Functional forms for $\vec{J}$ and $f$ are assumptions based off "constituitive laws".

A constituitive law is a measured or assumed mathematical relationship between physical quantities.

For instance, the ideal gas law

$$PV = nRT$$

may be viewed as a "constituitive law".

Generally for models there may be many different kinds of fluxes and sources so that (i) becomes

$$u_t = -\sum_{i=1}^{N} \vec{\nabla} \cdot \vec{J}_i + \sum_{j=1}^{M} f_j(\vec{x}, t, u)$$
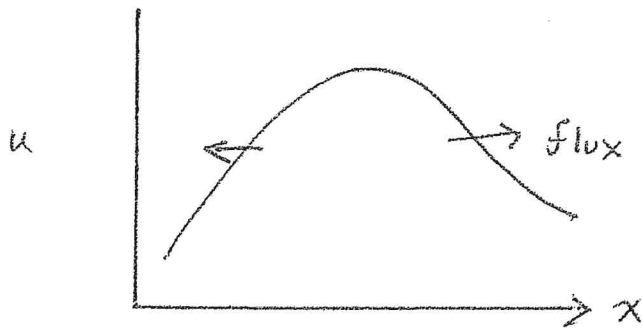
## EXAMPLE     Diffusion

Let $u$ = concentration of a substance

(1)     $$\vec{J} = -D\vec{\nabla}u \qquad \text{Fick's Law}$$

is an assumed law for the flux. Here $D$ is the <u>diffusivity</u> of the substance in the medium.

$$\vec{\nabla}u = \text{direction } u \uparrow \text{ most rapidly}$$

Thus flux in (1) indicates substance moves in direction $u$ decreasing most rapidly



In some media $D$ depends on $\vec{x}$.

Large molecules typically have a small $D$.

Spatial dependence of $D$ on $\vec{x}$ may be due to the medium is not homogeneous (perhaps stratified in some manner)

If one assumes $\vec{J} = -D(\vec{x})\vec{\nabla}u$ in the conservation equation we arrive at

$$(2) \qquad \frac{\partial u}{\partial t} = \vec{\nabla}\cdot(D(\vec{x})\vec{\nabla}u)$$

and when $D > 0$ is constant, eqn (2) becomes the <u>diffusion eqn</u>

$$(3) \qquad u_t = D\nabla^2 u \qquad\qquad \vec{x}\in\Omega, \; t > 0$$

with sources present

$$(4) \qquad u_t = D\nabla^2 u \; + \; f(\vec{x},t,u)$$

is a <u>reaction-diffusion equation</u>

## Remarks on units:

Let $M, L, T$ be mass, time and length.

$$[u] = ML^{-3}$$

$$[u_{xx}] = ML^{-5}$$

Thus since $[u_t] = [D][\nabla^2 u]$ we have

$$[D] = L^2 T^{-1}$$

$$[\vec{J}] = ML^{-2}T^{-1}$$

<u>EXAMPLE</u>    <u>Heat Eqn   (Thermal Transport)</u>

$$\vec{T}(\vec{x}, t) \quad = \text{ temperature} \qquad [T] = °$$

$$u(\vec{x}, t) \quad = \text{ energy density} \qquad [u] = J/m^3$$

$$\rho \quad = \text{ medium density} \qquad [\rho] = kg/m^3$$

$$C \quad = \text{ specific heat} \qquad [C] = J/(m{-}°)$$

$$K \quad = \text{ thermal conductivity} \quad [K] = J/(m\,sec\,°)$$
$$\text{of medium}$$

Most generally $\underline{K}$, $C$ and $\rho$ could depend on $\vec{x}$. For example the medium insular properties could vary.

Empirical (Constituitive) laws

$$u(\vec{x}, t) \equiv C\rho\, \vec{T}(\vec{x}, t)$$

$$\vec{J}(x, t) = -\underline{K}\,\vec{\nabla} T$$

in which case

$$C\rho\, \vec{T}_t = \nabla \cdot (\underline{K}\,\vec{\nabla} \vec{T}) + f$$

If $C, \rho, \underline{K}$ are constant

$$\frac{\partial \vec{T}}{\partial t} = D\,\nabla^2 T + F(\vec{x}, t, T) \quad, \quad \vec{x} \in \Omega$$

is a PDE whose solution yields the spatiotemporal variations of temperature

$$D = \frac{K}{C\rho} \qquad\qquad F = \frac{f}{C\rho}$$

<u>EXAMPLE</u>    <u>Advection/Diffusion</u>

$$\vec{J}_{Diff} = -D(x)\vec{\nabla}u \qquad\qquad \text{Diffusion}$$

$$\vec{J}_{Adv} = + u\,\vec{v}(\vec{x}) \qquad\qquad \text{Advection}$$

where $D$ = diffusivity and $\vec{v}(\vec{x})$ is the velocity of the fluid that $u$ is in.

Conservation of $u$ implies

$$u_t = \vec{\nabla}\cdot(D(x)\vec{\nabla}u) - \vec{\nabla}\cdot(\vec{v}\,u) + f$$

Is a reaction-diffusion-advection eqn.

If $D,$   are constant

$$u_t = D\nabla^2 u - \vec{v}\cdot\vec{\nabla}u + f$$

which in one dimensional spatial domain becomes

$$u_t = D u_{xx} - v u_x + f$$

<u>Remark</u>   For diffusion the " − " sign is needed for $u$ to move toward lower concentrations

For advection the " + " sign implies $u$ moves along with the fluid flow
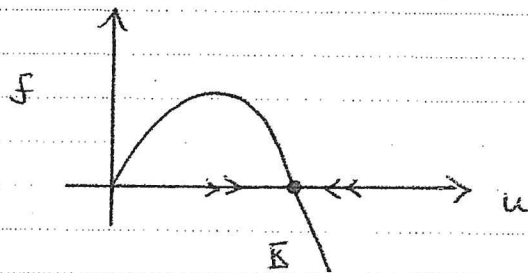
# EXAMPLE    Population Models

$$u(\vec{x}, t) = \text{population density at } \vec{x} \in \Omega.$$

Notion of density works better for bacteria or cells. Could be trees, etc.

## Logistic Source term

$$f(u) = ru\left(1 - \frac{u}{K}\right)$$

where $K$ = carrying capacity of environment.



Fact $f(u) < 0$ for $u > K$ meant to reflect death due to overcrowding (competition)

## Other source terms

Suppose a substance $c(\vec{x}, t)$ is the primary food source.

$$f = f(u, c)$$

may have the generic property $f_c > 0$ to reflect (bacterial) birth rate is higher if $c$ is larger. Perhaps

$$f(u, c) = k \frac{uc}{c + K} \qquad k, K \in \mathbb{R}$$

Constituitive laws for organism movement

$$\vec{J} = -D \vec{\nabla} u \qquad \text{Diffusive (random)}$$

$$\vec{J} = +u \vec{v} \qquad \text{Advection}$$

$$\vec{J} = +\alpha u \vec{\nabla} c \qquad \text{Chemotaxis}$$

$$\vec{J} = +\alpha u \vec{\nabla} T \qquad \text{Thermotaxis}$$

where $\vec{v}$ = fluid velocity, $c$ = food concentration, $T$ = temperature

Some bacteria are chemotactic. They tend to move toward food.

Slime mold and nematodes are thermotactic

MODEL ONE

$$\frac{\partial u}{\partial t} = D_1 \nabla^2 u + f_1(u, c)$$

$$\frac{\partial c}{\partial t} = D_2 \nabla^2 c + f_2(u, c)$$

Both organism and food diffuse through homogeneous medium.

$$f_1 > 0 \qquad \frac{\partial f_1}{\partial c} > 0$$

and $f_2$ reflects a loss of $c$ that $u$ eats.

## MODEL TWO    (Logistic)

$$\vec{J} = -D \vec{\nabla} u \qquad\qquad D \in \mathbb{R}^+ \text{ const.}$$

$$f = r u \left(1 - \frac{u}{K}\right)$$

yields in one spatial domain

$$u_t = D u_{xx} + r u \left(1 - \frac{u}{K}\right)$$

## MODEL THREE    (very slow fluid flow)

$$\vec{J}_1 = -D_1 \vec{\nabla} u \qquad\qquad D \in \mathbb{R}^+ \text{ const}$$

$$\vec{J}_2 = + \alpha u \vec{\nabla} c \qquad\qquad \alpha \in \mathbb{R}^+ \text{ const}$$

and certain source terms $f_k$. Conservation law implies

$$(1) \qquad \frac{\partial u}{\partial t} = -\vec{\nabla} \cdot \vec{J}_1 - \vec{\nabla} \cdot \vec{J}_2 + f_1$$

If $c$ merely diffuses we obtain coupled equations for $u, c$

$$(2) \qquad \frac{\partial u}{\partial t} = \underbrace{D_1 \vec{\nabla}^2 u}_{\text{diff}} - \underbrace{\alpha \vec{\nabla} \cdot (u \vec{\nabla} c)}_{\text{chemotaxis}} + f_1$$

$$(3) \qquad \frac{\partial c}{\partial t} = D_2 \vec{\nabla}^2 c \qquad\qquad + f_2$$

For $\Omega \subset \mathbb{R}$ eqn (2) would be

$$u_t = D_1 u_{xx} - \alpha (u c_x)_x + f_1$$

<u>EXAMPLE</u>    <u>Electro Diffusion</u>

Charged particles diffuse through
a medium having electric field
$\vec{E}(\vec{x})$.

$$u(\vec{x}, t) = \text{charge density}$$

<u>Ohmic flux law</u>

$$\vec{J} = z \sigma \vec{E} \qquad\qquad z = \text{valence}$$

and $\sigma$ is conductivity (generally a
matrix for anisotropic non homogeneous
media)

If the electric field is given by

$$\vec{E} = -\vec{\nabla} \phi$$

where $\phi$ is the electric potential
one obtains

$$\frac{\partial u}{\partial t} = \underbrace{D \nabla^2 u}_{\text{diff}} + \underbrace{z \sigma \nabla^2 \phi}_{\text{electric}}$$

The eqn for $\phi$ is obtained using Maxwell's
eqn. Steady state version is

$$0 = D \nabla^2 u + z \sigma \nabla^2 \phi$$

$$-\beta u = \nabla^2 \phi \qquad\qquad (\vec{\nabla} \cdot \vec{E} = 4\pi \rho)$$

for an appropriate constant $\beta$

## Steady States of PDEs

More generally the steady states $\bar{u}(x)$ of some PDE (system) is a time $t$ independent solution which satisfies all boundary conditions. Stability is a separate condition. By way of example:

$$u_t = u_{xx} \qquad x \in [0,1]$$

$$u_x(0,t) = 0 \qquad \text{no flux BC}$$

$$u_x(1,t) = 0 \qquad \text{no flux BC}$$

$$u(x,0) = f(x) \qquad \text{initial cond I.C.}$$

Associated problem for steady state $\bar{u}(x)$

$$0 = \bar{u}_{xx} \qquad x \in [0,1]$$

$$\bar{u}_x(0) = 0 \qquad \text{no-flux}$$

$$\bar{u}_x(1) = 0 \qquad \text{no-flux}$$

This is an ODE problem! The general solution of $\bar{u}_{xx} = 0$ is

$$\bar{u}(x) = Ax + B \qquad A, B \text{ constants}$$

Find A using B.C.

$$\bar{u}'(x) = A$$

$$\bar{u}'(0) = A = 0$$

Hence

$$\boxed{\bar{u}(x) = B}$$

This also satisfies the other B.C. $\bar{u}'(1) = 0$.
But, we don't know B yet.

Recall that

$$M(t) = \int_0^1 u(x,t)\,dx$$

is the total amount of $u(x,t)$ in the
domain $[0,1]$. Since the B.C. are
no flux at both end points (boundary),
$M(t)$ must remain constant. Hence

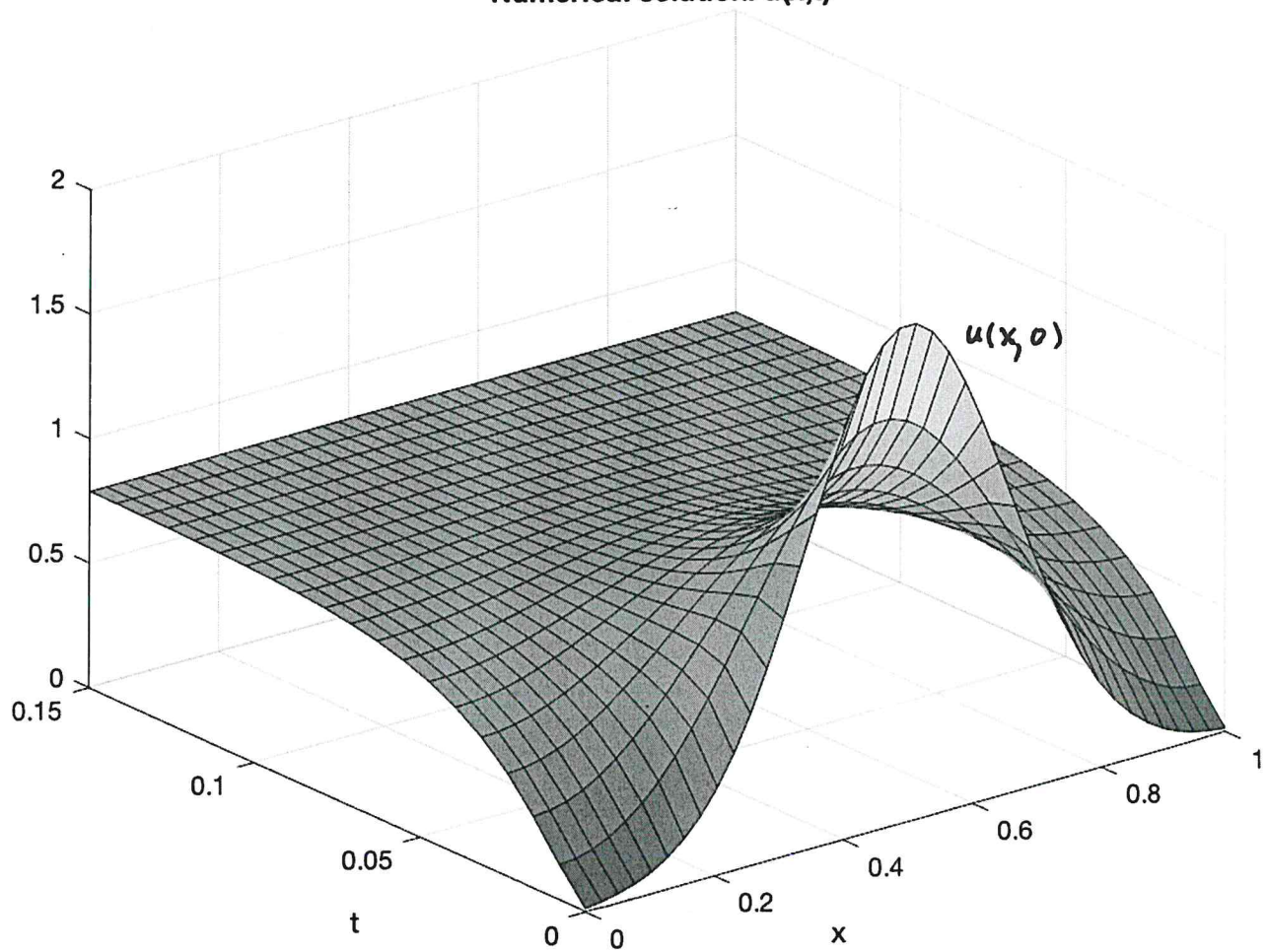$$M(0) = \int_0^1 \bar{u}(x)\,dx = \int_0^1 u(x,0)\,dx$$

For the initial condition

$$u(x,0) = 2\exp\left(-(x-\tfrac{1}{2})^2 / 0.05\right)$$

we find $\bar{u}(x) = B$ where

$$\boxed{B = \int_0^1 u(x,0)\,dx \approx 0.79}$$

**Numerical solution: u(x,t)**

$u(x, 0)$

$$u_t = u_{xx}$$
$$u_x(0, t) = 0$$
$$u_x(1, t) = 0$$

} Both no-flux
Boundary Conditions

```matlab
%   Heat equation with Neumann BC on [0,1]
%
function pdex01
m = 0;
x = linspace(0,1,40);          x ∈ [0,1]
t = linspace(0,0.15,20);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
% Extract the first solution component as u.
u = sol(:,:,1);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Surface plot of u(x,t)
surf(x,t,u)
title('Numerical solution: u(x,t)')
xlabel('x')
ylabel('t')
% Solution profile u(x,*) at last time.
figure
plot(x,u(end,:))
title('u(x,t) at t = 0.15')
xlabel('x')
ylabel('u(x,0.15)')
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%               Defining the problem (m=0)
%
%   c(x,t,u,u_x) u_t = (f(x,t,u,u_x))_x + s(x,t,u,u_x)
%
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1;
f = 1*DuDx;
s = 0;
%           u(x,0)=u0(x)
%
function u0 = pdex1ic(x)
u0=2*exp(-(x-0.5)^2/(0.05));
%
%          p + q*f = 0                 x=xl,xr
%
%   where f is the flux f declared in the PDE above
%
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = 0;
qr = 1;
```

Handwritten annotations:

$x \in [0,1]$

$u(x,0) = A \exp\left(-(x-x_0)^2/\sigma^2\right)$

$u_x(0,t) = 0$

$u_x(1,t) = 0$

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**EXAMPE**    Find the steady state of

$$u_t = u_{xx}$$

$$u(0,t) = 0 \qquad \text{Dirichlet}$$

$$u_x(1,t) = 0 \qquad \text{Neumann (no-flux)}$$

$$u(x,0) = \sin(\pi x)$$

Steady state problem

$$\bar{u}_{xx} = 0 \qquad \bar{u}(0) = 0 \qquad \bar{u}'(1) = 0$$
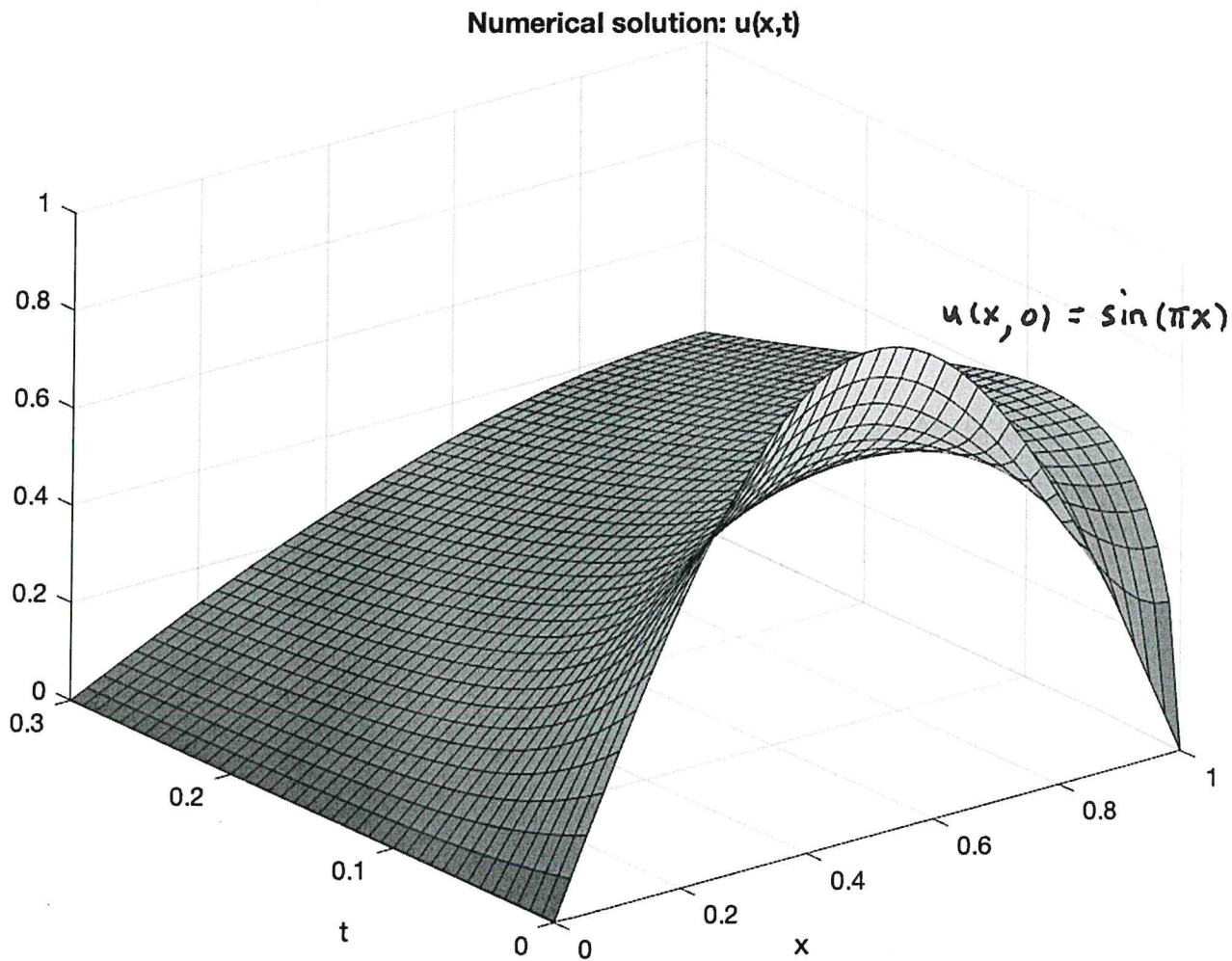
General Soln

$$\bar{u}(x) = Ax + B$$

Use B.C.

$$\bar{u}(0) = B \qquad = 0$$

$$\bar{u}'(1) = A \qquad = 0$$

Conclude

$$\bar{u}(x) = 0$$

**Numerical solution: u(x,t)**

$u(x,0) = \sin(\pi x)$

$$u_t = u_{xx}$$
$$u(0,t) = 0$$
$$u_x(1,t) = 0$$

Dirichlet B.C.
no-flux B.C.

```matlab
%  Heat equation with Neumann BC on [0,1]
%
function pdex02
m = 0;
x = linspace(0,1,40);        x ∈ [0,1]
t = linspace(0,0.30,40);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
% Extract the first solution component as u.
u = sol(:,:,1);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Surface plot of u(x,t)
surf(x,t,u)
title('Numerical solution: u(x,t)')
xlabel('x')
ylabel('t')
% Solution profile u(x,*) at last time.
figure
plot(x,u(end,:))
title('u(x,t) at t = 0.15')
xlabel('x')
ylabel('u(x,0.15)')
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%              Defining the problem (m=0)
%
%    c(x,t,u,u_x) u_t = (f(x,t,u,u_x))_x + s(x,t,u,u_x)
%
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1;
f = 1*DuDx;
s = 0;
%            u(x,0)=u0(x)
%
function u0 = pdex1ic(x)
u0=sin(pi*x);                u(x,0) = sin(πx)
%
%          p + q*f = 0                x=xl,xr
%
%   where f is the flux f declared in the PDE above
%
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = ul;           } u(0,t) = 0
ql = 0;
pr = 0;            } u_x(1,t) = 0
qr = 1;
```

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