Advection-Diffusion

D. Gurarie

Flux-divergence

Mass conservation law for space-time density $u(x,t)$ and flux $\mathbf{J} = \mathbf{J}(u, \nabla u, ...)$ gives PDE

$$u_t = \nabla \cdot \mathbf{J} + S \tag{1}$$

Here gradient $\nabla = (\partial_x, \partial_y, ...)$, S – local sources/sinks. PDE (1)is derived from integral form: total mass in volume V, $m = \iint_D u dx$, has rate of change

$$\frac{d}{dt} m = \iint_V u_t dx = \oint_\Sigma \mathbf{J} \cdot N ds \tag{2}$$

- total flux through the boundary (Fig. 1). Since (2) holds for any (small) volume V, we get PDE (1) by divergence Theorem applied to the RHS of (2).

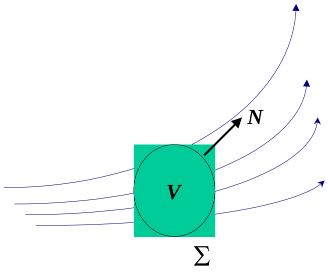

Figure 1

Advective (transport) flux is a function of *u* alone,

$$\mathbf{J}_A = \mathbf{c}(u); \text{ or } \mathbf{c}u$$

c – velocity field, while diffusive flux depend on gradient

$$\mathbf{J}_D = D\nabla u; \text{ or } D \cdot \nabla u = \sum_j D_{ij} \partial_j u$$

D – diffusivity (scalar or tensor/matrix).

Specific cases

- 1D: $u_t = -cu_x + Du_{xx} + S$, on R or interval [a,b]
- nD: $u_t = -\mathbf{c} \cdot \nabla u + D\nabla^2 u + S$, on R^n or finite domain V (Fig.1)
- Polar coordinates (r,θ):

$$\nabla \cdot \mathbf{J}_A = c_r u_r + \frac{c_\theta}{r} u_\theta$$
$$\nabla \cdot \mathbf{J}_D = D\nabla^2 = D\left(u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta} \right)$$

- Spherical coordinates $(r,\theta,\phi): 0 < \theta < \pi$ - latitude; $0 < \phi < 2\pi$ - longitude:

$$\nabla \cdot \mathbf{J}_A = c_r u_r + \frac{1}{r}\left(c_\theta u_\theta + \frac{c_\phi u_\phi}{\sin\theta} \right)$$
$$\nabla \cdot \mathbf{J}_D = D\nabla^2 = D\left[u_{rr} + \frac{2}{r} u_r + \frac{1}{r^2}\left(u_{\theta\theta} + \frac{\cos\theta}{\sin\theta} u_\theta + \frac{u_{\phi\phi}}{\sin^2\theta} \right) \right]$$

Boundary conditions

Basic types of boundary conditions (BC) include on space-time cylinder (Fig.2)

	1D on [*0,l*]	nD in region V, Σ
Dirichlet (D)	$u\|_{x=0,l} = 0$ or $B_{0,1}$	$u\|_\Sigma = 0; B(y)$
Neumann (N)	$-u'\|_{x=0} = 0\ ;\ B_0$ $u'\|_{x=l} = 0\ ;\ B_1$	$\partial_n u\|_\Sigma = 0; B(y)$
Mixed (Robin)	$-\alpha_0 u' + \beta_0 u\|_{x=0} = 0\ ;\ B_0$ $\alpha_1 u' + \beta_1 u\|_{x=l} = 0\ ;\ B_1$	$(\alpha\partial_n u + \beta u)\|_\Sigma = 0; B(y)$

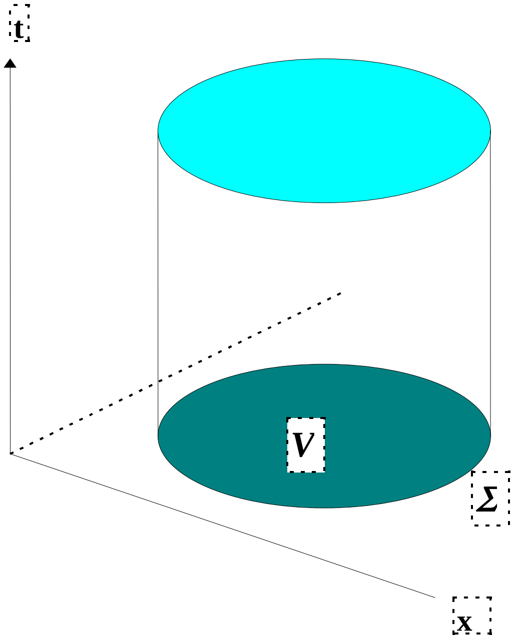

Figure 2

Initial condition (IC) for parabolic equation (1) is given by $u(x,0)=f(x)$ - initial density profile.

Solution methods

Free space problem (IVP) on R or R^n

$$\begin{cases} u_t=-cu_x+Du_{xx}+S;\ \text{or } u_t=-\mathbf{c}\cdot\nabla u+D\nabla^2 u+S \\ u(x,0)=f(x) \end{cases} \tag{3}$$

All cases (constant c,D) IVP-solution can be expressed through the fundamental Gaussian

$$G(x,t)=\frac{1}{(4\pi Dt)^{n/2}}e^{-x^2/4Dt} \tag{4}$$

Table 1

Case	*u(x,t)*
$c=0; S=0$	$\int_{\mathbf{R}^n} G(x-\xi,t)\,f(\xi)\,d\xi$
$c=0; S\neq 0$	$\int_0^t\int_{\mathbf{R}^n} G(x-\xi,t-\tau)\,S(\xi,\tau)\,d\xi d\tau$
$c\neq 0; S=0$	$\int_{\mathbf{R}^n} G(x-\mathbf{c}t-\xi,t)\,f(\xi)\,d\xi$

BVP in finite region: Eigenfunction expansion method

1D Diffusion with Dirichlet BC (and possible dissipation /loss rate of u)

$$\begin{cases} u_t = Du_{xx} - au + S;\ \text{on } [0,l] \\ \text{BC}: u|_{x=0,l} = 0 \\ \text{IC}: u(x,0) = f(x) \end{cases} \tag{5}$$

System of eigenvalues and eigenfunctions for BVP (5) consists of sin-Fourier modes

$$\begin{aligned} &\lambda_k = D\left(\frac{\pi k}{l}\right)^2 + a; \\ &\psi_k(x) = \sin\left(\frac{\pi k x}{l}\right); k = 1, 2, \ldots \end{aligned} \tag{6}$$

Any function f(x) on [0,l] can be expended in eigenmodes to get sin-Fourier series

$$\begin{aligned} &f(x) = \sum_1^\infty f_k \psi_k(x) \\ &f_k = \frac{2}{l}\int_0^l f(x)\psi_k(x)\,dx = \frac{\langle f|\psi\rangle}{\|\psi\|^2} \text{ - Fourier coefficients} \end{aligned}$$

Solution of (5) is given by eigenfunction (Fourier) expansion

$$u(x,t) = \sum_1^\infty f_k e^{-\lambda_k t}\psi_k(x) \tag{7}$$

As all $\lambda_k > 0$ (with or w/o dissipation), all IVP solutions decay exponentially,

$$u(x,t) < Ce^{-\lambda_1 t}; \lambda_1 = D\left(\frac{\pi}{l}\right)^2 + a$$

Solution of source problem $S(x,t)$ has similar expansion

$$\begin{aligned} &u(x,t) = \sum_1^\infty \left[\int_0^t e^{-\lambda_k(t-\tau)} S_k(\tau)\,d\tau\right]\psi_k(x) \\ &S_k(t) = \frac{\langle S|\psi_k\rangle}{\|\psi_k\|^2} \text{ - Fourier coefficient of } S \end{aligned} \tag{8}$$

For stationary source $S(x) = \sum S_k \psi_k(x)$, all terms of (8) can be integrated to get

$$u(x,t)=\sum_{1}^{\infty} S_k \frac{\left(1-e^{-\lambda_k t}\right)}{\lambda_k}\psi_k(x)\to w(x)+O\left(e^{-\lambda_1 t}\right)$$

Such solutions approach stable equilibrium:

$$w(x)=\sum_{1}^{\infty}\frac{S_k}{\lambda_k}\psi_k(x) \tag{9}$$

The equilibrium can be computed directly from stationary problem (5).

For boundary-source problem

$$\begin{aligned}&-Dw''+aw=0;\ \text{on } [0,l]\\ &w(0)=A; w(l)=B\end{aligned} \tag{10}$$

we get

$$\begin{aligned}w(x)&=\frac{A(l-x)+Bx}{l};\ \text{if } a=0\\ w(x)&=\frac{A\sinh\sqrt{a}(l-x)+B\sinh\sqrt{a}x}{\sinh\sqrt{a}l};\ \text{if } a>0\end{aligned}$$

Equilibrium solution (9) with stationary $S(x)$, has another ***integral representation*** through the fundamental solution (Green's function) of BVP,

$a=0$	$K(x,\xi)=\frac{1}{l}\begin{cases}x(l-\xi);x<\xi\\ \xi(l-x);x>\xi\end{cases}$
$a\neq 0$	$K(x,\xi)=\frac{1}{q(l)}\begin{cases}q(x)q(l-\xi);x<\xi\\ q(\xi)q(l-x);x>\xi\end{cases};$ $q(x)=\sinh\sqrt{a}x$

Namely,

$$w(x)=\int_0^l K(x,\xi)S(\xi)d\xi$$

Remark: The eigenfunction expansion method (shown for Dirichlet BC) extends to other types of 2-point BVP, e.g. Neumann, mixed. For Neumann BVP the eigensystem consists of cos-Fourier modes

$$\psi_k(x) = \cos\left(\frac{\pi k x}{l}\right); k = 0,1,2\ldots$$

and zero mode (k=0) corresponds to constant equilibrium density $w(x) = \psi_0(x) = 1$.

However, if transport term cu_x is added in any 2-point BVP, there is no more a "natural" eigenfunction system, and solution exhibit singular behavior at the boundaries!

Periodic problem in space

The "natural domain" for periodic functions in x "is a circle. In this case one can use both methods:

1) Fundamental solution, like on R or R^n
2) Fourier expansion method $\{e^{ikx} : k = -\infty, \infty\}$, or $\{\cos kx, \sin kx : k = 0,1,\ldots\}$ on $[-\pi, \pi]$

The Fourier modes are "eigenfunctions" of the derivative operators $L = \partial_x;\ L_2 = a\partial_x{}^2$, or $L_3 = a\partial_x{}^2 + b\partial_x + c$

$$\begin{aligned} L\left[e^{ikx}\right] &= ike^{ikx} \\ L_2\left[e^{ikx}\right] &= -k^2 e^{ikx} \\ L_3\left[e^{ikx}\right] &= \left(-ak^2 + ikb + c\right)e^{ikx} \end{aligned}$$

So Fourier series expansion of periodic BVP

$$\begin{aligned} &u_t = Du_{xx} - cu_x + au + S; \\ &\text{BC: } u(0,t) = u(2\pi,t); \end{aligned} \qquad (11)$$

on circle is given by

$$u(x,t) = \mathrm{Re}\left\{\sum_{-\infty}^{\infty}\left[f_k e^{\lambda_k t} + \int_0^t e^{\lambda_k(t-\tau)} S_k(\tau)\right]e^{ikx}\right\} \qquad (12)$$

with complex eigenvalues $\lambda_k = -Dk^2 + ick + a$.

To get fundamental solution $G(x,t)$ on circle we use the so-called *theta-function* ("circular Gaussian")

$$\theta(q,z) = 1 + 2\sum_1^\infty q^{k^2}\cos(2kz)$$

Then

$$G(x,t) = \frac{1}{2\pi}\sum_{-\infty}^{\infty} e^{-tk^2+ikx}\,\frac{1}{2\pi}\left(1+2\sum_1^\infty e^{-tk^2}\cos kx\right) = \theta\left(e^{-t}, x/2\right) \tag{13}$$

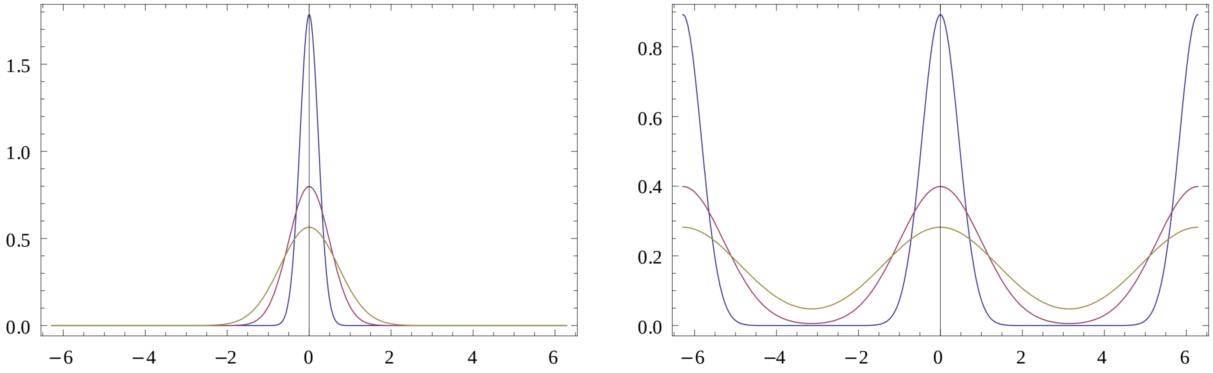

Fig.3: Standard Gaussian (left) and circular Gaussian (13) – right

Having computed we can write solution (12) as convolution integral on circle (similar to Table 1)

$$u(x,t) = \underbrace{\int_0^{2\pi} G(x-ct-\xi,t)\,f(\xi)}_{IVP} + \underbrace{\int_0^t\int_0^{2\pi} G(x-ct-\xi,t-\tau)\,S(\xi,\tau)d\xi d\tau}_{\text{source}}$$