

# List of pdfcomments

# Notes on the Diffusion Equation

Thursday 28<sup>th</sup> November, 2013

## 1 Introduction

Consider an arbitrary solution  $u : \mathbb{X} \times \mathbb{T} \mapsto \mathbb{R}$  to the simple diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}. \quad (1)$$

A computationally feasible approach would be to first establish  $|\mathbb{J}|$  discrete grid-points,  $\vec{X} = [X_j]_{j \in \mathbb{J}}$ , and thence partition the spatial domain  $\mathbb{X}$  into contiguous intervals  $\mathbb{I}_j := (X_{j-1}, X_j]$ . The coarse dynamics at the grid-points are then summarised by  $\vec{U} = [U_j]_{j \in \mathbb{J}}$ , where  $U_j(t) = u(X_j, t)$  for all  $t \in \mathbb{T}$ , according to some temporal evolution

$$\dot{\vec{U}}(t) = \vec{g}(\vec{U}(t)). \quad (2)$$

Consequently, a link from the coarse dynamics  $\vec{U}$  back to the continuum dynamics  $u$  might be provided by choosing an appropriate spatial mapping of the form

$$u := u(x, \vec{U}(t)). \quad (3)$$

Under this scheme, the linear diffusion equation (1) becomes

$$\frac{\partial u}{\partial \vec{U}} \cdot \vec{g} = \frac{\partial^2 u}{\partial x^2}. \quad (4)$$

Observe that the evolution of  $u$  now has nonlinear interactions with  $\vec{U}$ .

## 2 Centre Manifold Approximation

The original diffusion equation (1) admits eigensolutions of the form

$$u(x, t) = e^{\lambda t \pm \sqrt{\lambda} x}, \quad (5)$$

which are physically realisable for real eigenvalues  $\lambda = -k^2 \leq 0$  for corresponding eigenmode wavenumbers  $\pm k$ . As a consequence, the transient solutions corresponding to  $\lambda < 0$  decay rapidly to the centre manifold corresponding to  $\lambda = 0$ .

This centre manifold can be found in practice by iteratively refining approximations to  $u$ . In particular, consider a series expansion of the form

$$u \sim \hat{u}_0 + \gamma \hat{u}_1 + \gamma^2 \hat{u}_2 + \dots, \quad (6)$$

for some parameter  $0 \leq \gamma \leq 1$ . Now, the constant eigensolution for  $\lambda = 0$  implies a slow evolution for the coarse dynamics given by equation (2), which therefore admits a series expansion of the form

$$\dot{\vec{U}} \sim \gamma \vec{g}_1 + \gamma^2 \vec{g}_2 + \dots. \quad (7)$$

Hence, equation (4) may be decomposed at each order  $\ell$  of the parameter  $\gamma$ , giving

$$\frac{\partial^2 \hat{u}_0}{\partial x^2} = 0, \quad (8)$$

$$\frac{\partial^2 \hat{u}_\ell}{\partial x^2} = \sum_{m=0}^{\ell-1} \frac{\partial \hat{u}_m}{\partial \vec{U}} \cdot \vec{g}_{\ell-m}, \quad \text{for } \ell = 1, 2, \dots. \quad (9)$$

## 3 Leading Approximation

The leading equation (8) admits any spatially piecewise linear function as a solution. Hence, in keeping with the discretisation imposed by the coarse dynamics, consider the linear approximation

$$\hat{u}_0 = \sum_{j \in \mathbb{J}} \chi_j (\xi_j U_j + (1 - \xi_j) U_{j-1}), \quad (10)$$

with indicator  $\chi_j(x) = 1$  (or 0) for  $x \in \mathbb{I}_j$  (or  $x \notin \mathbb{I}_j$ ), and interpolator  $\xi_j(x) = \frac{x - X_{j-1}}{X_j - X_{j-1}}$ . This particular approximation is chosen to be continuous

across the boundaries of each interval  $\mathbb{I}_j$ . In general, it suffices to impose a continuity condition at the right-hand end of each  $\mathbb{I}_j$ , namely:

$$[u]_j := \lim_{\epsilon \rightarrow 0^+} u(X_j + \epsilon, t) - u(X_j - \epsilon, t) = 0. \quad (11)$$

Unfortunately, this linear approximation is not smooth at the interval boundaries. For convenience, consider regular grid spacings of size  $X_j - X_{j-1} = H$ . Then, denoting  $\partial u / \partial x$  as  $u'$ , observe that

$$[\hat{u}'_0]_j = \frac{1}{H}(U_{j+1} + U_{j-1} - 2U_j) = \frac{1}{H} \delta^2 \hat{u}_0|_{X_j}, \quad (12)$$

for the centred difference  $\delta u(x, t) := u(x + \frac{H}{2}, t) - u(x - \frac{H}{2}, t)$ . However, this non-smoothness may be corrected at higher order by imposing a further internal boundary condition, namely

$$[u']_j = \frac{1 - \gamma}{H} \delta^2 u|_{X_j}. \quad (13)$$

Consequently, smooth approximations are found in the limit as  $\gamma \rightarrow 1$ .

## 4 Linear Eigenmode Analysis

Consider a single eigenmode of the form (5) for some fixed, non-dimensionalised wavenumber  $\kappa = kH > 0$ . Thus, allowing for the partitioning of  $\mathbb{X}$ , let

$$u \sim \sum_{j \in \mathbb{J}} \chi_j a_j e^{i\kappa \xi_j} + \text{c.c.}, \quad (14)$$

for arbitrary, time-varying, complex coefficients  $a_j = A_j + iB_j$ . We now seek the ‘spatial’ evolution from interval to interval for the given wavenumber. The continuity condition (11) implies that

$$a_{j+1} - a_j e^{i\kappa \xi_j} + \text{c.c.} = 0. \quad (15)$$

Similarly, the smoothness condition (13) implies that

$$ika_{j+1} - ika_j e^{i\kappa} + \text{c.c.} = \frac{1 - \gamma}{H} (a_{j+1} e^{i\kappa} + a_j - 2a_j e^{i\kappa}) + \text{c.c.}, \quad (16)$$

where continuity has also been invoked at the left-hand of the  $j$ th interval. In coefficient form, the update from the  $j$ th to  $(j + 1)$ th segment is

$$\begin{bmatrix} 1 & 0 \\ fc & 1 - fs \end{bmatrix} \begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix} = \begin{bmatrix} c & -s \\ s + f(2c - 1) & c - 2fs \end{bmatrix} \begin{bmatrix} A_j \\ B_j \end{bmatrix}, \quad (17)$$

where  $c + is := e^{i\kappa}$  and  $f := \frac{1-\gamma}{\kappa}$ . Now, letting  $a_{j+1} = \mu a_j$ , the characteristic equation for the growth factor  $\mu$  is

$$(1 - fs) \left[ \mu^2 - 2 \frac{c - fs}{1 - fs} \mu + 1 \right] = 0, \quad (18)$$

with roots given by

$$\mu = \beta \pm \sqrt{\beta^2 - 1} \quad \text{for } \beta = \frac{c - fs}{1 - fs}. \quad (19)$$

Observe that  $\beta \leq 1$  since  $c = \cos \kappa \leq 1$  and  $1 - fs = 1 - (1 - \gamma) \frac{\sin \kappa}{\kappa} \geq 0$ . Thus, for  $|\beta| < 1$ , the factors are complex with magnitude  $|\mu| = 1$ , indicating marginally stable evolution of  $a_j$ . This includes the limiting case of  $\gamma = 1$  ( $f = 0$ ), for which  $\mu = c \pm is = e^{\pm i\kappa}$ . Likewise,  $\mu = \pm 1$  for  $\beta = \pm 1$ , corresponding to  $\kappa = n\pi$ ,  $n = 0, 1, 2, \dots$ . Finally, for small regions near each  $\kappa = (2n + 1)\pi$ , it is found that  $\beta < -1$ , resulting in two real factors,  $\mu < -1$  and  $-1 < \mu < 0$ , indicating unstable (saddle) evolution. More precisely, these unstable regions occur when

$$\frac{\kappa}{2} < (1 - \gamma) \tan \frac{\kappa}{2}, \quad \kappa \neq n\pi. \quad (20)$$

Thus, at equilibrium ( $\gamma = 0$ ) there is an initial forbidden gap  $\kappa \in (0, \pi)$  adjacent to the centre manifold wavenumber  $\kappa = 0$  (see Figure 1), indicating that transient solutions decay to the centre manifold at a rate of at least  $\lambda = -\frac{\kappa^2}{H^2} = -\frac{\pi^2}{H^2}$ . It is this gap that provides robustness to nonlinear perturbations of the system about the equilibrium.

## 5 Linear Dual Space

Suppose the domain  $\mathbb{X}$  has been discretised to have outer boundaries  $X_{\underline{J}}$  and  $X_{\bar{J}}$  for indices  $\underline{J} = \inf \mathbb{J}$  and  $\bar{J} = \sup \mathbb{J}$ . Assume for convenience that  $|\mathbb{J}| > 2$ . Then an appropriate inner product for spatially square-integrable fields  $u$  and  $v$  is given by

$$\langle u, v \rangle = \int_{X_{\underline{J}}}^{X_{\bar{J}}} uv \, dx = \sum_{j=\underline{J}+1}^{\bar{J}} \int_{\mathbb{I}_j} uv \, dx. \quad (21)$$

It can then be shown, for twice-differentiable fields, that

$$\langle u'', v \rangle = \langle u, v'' \rangle + R, \quad (22)$$

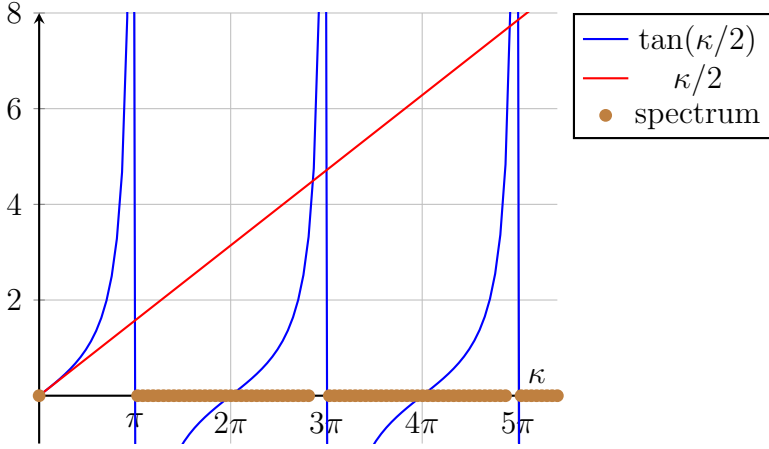


Figure 1: The equilibrium spectrum determined by the forbidding condition (20).

with residual

$$R = \sum_{j=\underline{J}+1}^{\bar{J}} [r]_{X_{j-1}}^{X_j} = r_{\bar{J}} - r_{\underline{J}} - \sum_{j=\underline{J}+1}^{\bar{J}-1} [r]_j, \quad (23)$$

for  $r = u'v - v'u$ . Now, assuming that both  $u$  and  $v$  obey conditions (11) and (13), the residual jump at  $X_j$  becomes

$$\begin{aligned} [r]_j &= [u']_j V_j - [v']_j U_j \\ &= \frac{1-\gamma}{H} [(U_{j+1} + U_{j-1})V_j - (V_{j+1} + V_{j-1})U_j]. \end{aligned} \quad (24)$$

Observe that terms from adjacent intervals  $\mathbb{I}_{j-1}$  and  $\mathbb{I}_{j+1}$  will cancel terms from  $\mathbb{I}_j$ , leaving only contributions from the outermost boundary intervals  $\mathbb{I}_{\underline{J}+1}$  and  $\mathbb{I}_{\bar{J}}$ ; consequently:

$$\begin{aligned} R &= u'_{\bar{J}} V_{\bar{J}} - v'_{\bar{J}} U_{\bar{J}} - u'_{\underline{J}} V_{\underline{J}} + v'_{\underline{J}} U_{\underline{J}} \\ &\quad - \frac{1-\gamma}{H} [U_{\bar{J}} V_{\bar{J}-1} - V_{\bar{J}} U_{\bar{J}-1} + U_{\underline{J}} V_{\underline{J}+1} - V_{\underline{J}} U_{\underline{J}+1}]. \end{aligned} \quad (25)$$

On a finite domain, there are three main outer boundary conditions that lead to a zero residual:

**periodic** Having period  $\bar{J} - \underline{J}$  corresponds to  $U_{\bar{J}} = U_{\underline{J}}$ . Furthermore, by joining the domain cylindrically at  $X_{\underline{J}}$  and  $X_{\bar{J}}$ , it can be shown that

$$u'_{\underline{J}} - u'_{\bar{J}} = [u']_{\bar{J}} = \frac{1-\gamma}{H} (U_{\underline{J}+1} + U_{\bar{J}-1} - 2U_{\bar{J}}), \quad (26)$$

using condition (13). Hence,  $R = 0$  if correspondingly  $v$  is periodic with period  $\bar{J} - \underline{J}$ .

**Dirichlet** Setting  $u = 0$  at the boundaries corresponds to  $U_{\underline{J}} = U_{\bar{J}} = 0$ , giving  $R = 0$  if correspondingly  $v = 0$  on the boundaries.

**Neumann** Requiring  $u' = 0$  on the boundaries (for  $\gamma = 1$ ) corresponds to

$$u'_{\underline{J}} = \frac{1-\gamma}{H}(U_{\underline{J}+1} - U_{\underline{J}}), \quad u'_{\bar{J}} = \frac{1-\gamma}{H}(U_{\bar{J}} - U_{\bar{J}-1}), \quad (27)$$

giving  $R = 0$  if correspondingly  $v' = 0$  on the boundaries.

Under any of the above three conditions, observe that  $\langle \mathcal{L}u, v \rangle = \langle u, \mathcal{L}v \rangle$  for  $\mathcal{L} = \partial^2/\partial x^2$ , and hence  $\mathcal{L}$  is self-adjoint. Furthermore, we are free to choose any dual  $v$ , e.g. to satisfy  $\mathcal{L}v = 0$  for convenience. In particular, we may specifically target the  $j$ -th interval for  $u$ , for each  $j \in \mathbb{J}$ , with  $v = \hat{v}_0^{[j]}$ , where

$$\hat{v}_0^{[j]} = \chi_j \xi_j + \chi_{j+1}(1 - \xi_{j+1}), \quad (28)$$

which satisfies conditions (11) and (13) for  $\gamma = 0$ . It can then be shown in general that

$$\langle u'', \hat{v}_0^{[j]} \rangle = -[u']_j + \frac{1}{H} \delta^2 u|_{X_j}, \quad (29)$$

for any continuous, twice-differentiable  $u$ .

## 6 First-order Approximation

Substituting the leading approximation (10) into the nonlinear diffusion equation (9) for  $\ell = 1$  results in the first-order equation

$$\hat{u}_1'' = \sum_{j \in \mathbb{J}} \chi_j (\xi_j g_{1,j} + (1 - \xi_j) g_{1,j-1}). \quad (30)$$

Spatial integration then gives

$$\hat{u}_1' = \frac{H}{2} \sum_{j \in \mathbb{J}} \chi_j (\xi_j^2 g_{1,j} - (1 - \xi_j)^2 g_{1,j-1} + c_{1,j}), \quad (31)$$

$$\hat{u}_1 = \frac{H^2}{6} \sum_{j \in \mathbb{J}} \chi_j (\xi_j^3 g_{1,j} + (1 - \xi_j)^3 g_{1,j-1} + 3\xi_j c_{1,j} + d_{1,j}). \quad (32)$$

Recall from the chosen spatial discretisation that  $u|_{X_j} = U_j$  at each grid-point. Observe this is already satisfied by  $\hat{u}_0$  from equation (10), implying from expansion (6) that

$$\hat{u}_\ell|_{X_j} = 0 \quad \text{for } \ell = 1, 2, \dots \quad (33)$$

Thus  $[\hat{u}_\ell]_j = 0$ , satisfying the continuity condition (11), and  $\delta^2 \hat{u}_\ell|_{X_j} = 0$ . Now, evaluating equation (32) at  $\xi_j = 0$  gives  $d_{1,j} = -g_{1,j-1}$ , and at  $\xi_j = 1$  gives  $3c_{1,j} = -(g_{1,j} - g_{1,j-1})$ . Thus, from equation (31), observe that

$$[\hat{u}'_1]_j = -H\left(1 + \frac{1}{6}\delta^2\right)g_{1,j}. \quad (34)$$

However, the smoothness condition (13) gives

$$[\hat{u}'_1]_j = \frac{1}{H} \delta^2 \hat{u}_1|_{X_j} - \frac{1}{H} \delta^2 \hat{u}_0|_{X_j} = -\frac{1}{H} \delta^2 U_j, \quad (35)$$

and hence

$$\left(1 + \frac{1}{6}\delta^2\right)g_{1,j} = \frac{1}{H^2} \delta^2 U_j. \quad (36)$$

This solution can also be obtained more directly via the dual space by computing  $\langle \hat{u}''_1, \hat{v}_0^{[j]} \rangle$  from equations (28) and (30), and using results (29) and (35).