Rational modelling determines boundary conditions

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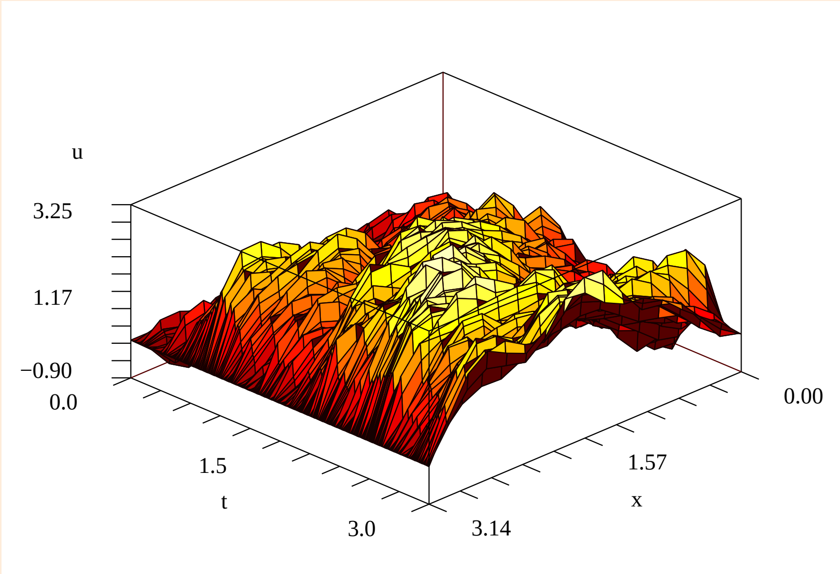

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1 Introduce modelling a toy

Consider the nonlinear diffusion of $u(x,t)$: <simtoy>

$$\frac{\partial u}{\partial t} = u\frac{\partial^2 u}{\partial x^2}\,, \quad \text{such that} \quad u = 0 \text{ on } x = \pm 1\,.$$

The decaying parabola $u = u_0(1-x^2)/(1+2u_0t)$ emerges quickly.

Show route from fudged problem to this solution is feasible.

Fudge the boundary conditions ...

For $\gamma = 1$ this is the same BC:

$$2\gamma u = \pm(1-\gamma)\frac{\partial u}{\partial x} \quad \text{on } x = \pm 1\,.$$

For any γ the decaying parabola $u = u_0(1-\gamma x^2)/(1+2\gamma u_0 t)$ emerges.

Exercise: deduce similar result when the 2 on the left is replaced by an 'Euler parameter' E.

. . . and a centre manifold appears

- When $\gamma = 0$ the BCs $2\gamma u = \pm(1-\gamma)u_x$ are insulating $\Rightarrow u = u_0$, constant, is attractive set of equilibria.
- Decay rates $\lambda \approx 0, -2.5u_0, -10u_0, -23u_0, \ldots$ $\Rightarrow$ *centre manifold* exists parametrised by u_0 and γ:

$$u(x,t) = (1-\gamma x^2)u_0 \quad \text{such that} \quad \dot{u}_0 = -2\gamma u_0^2\,.$$

Recovers earlier solution when $\gamma = 1$, via theory based upon $\gamma = 0$.

Relevant: all initial conditions approach model

For all solutions $u(x,t)$, there exits an initial $u_0(0)$ s.t.

$$\|u(x,t)-(1-\gamma x^2)u_0(t)\| = \mathcal{O}(e^{-\beta t}) \quad \text{as } t\to\infty\,.$$

This guarantees quick attraction to dynamics of model $\dot u_0 = -2\gamma u_0^2\,.$

Draw set of all states with same long-term evolution

<isochron>

Summary *creatively manipulate the BCs to obtain this model, via resolving structures within the domain.*

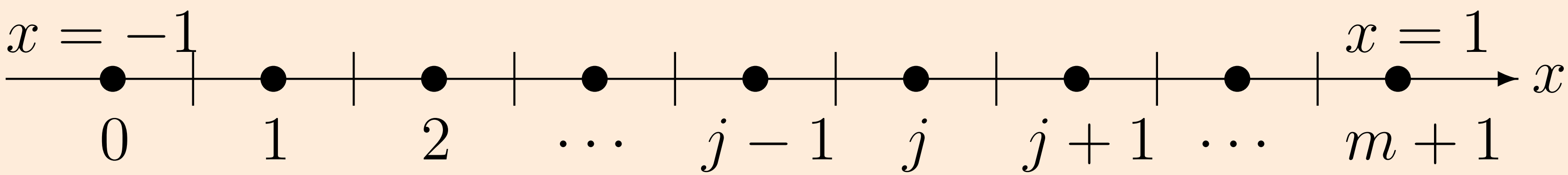
2 Boundary conditions for discretisations

Continue with the example nonlinear diffusion of $u(x,t)$:

$$\frac{\partial u}{\partial t} = u\frac{\partial^2 u}{\partial x^2}\,, \quad \text{such that} \quad u = 0 \text{ on } x = \pm 1\,.$$

Now divide the domain into m finite sized elements.

by artificially introducing *internal boundary conditions* (IBCs).



Let $u = v_j(x,t)$ be the field in the jth element, then

$$\left.\frac{\partial v_j}{\partial x}\right|_{x_j-h/2} = \left.\frac{\partial v_j}{\partial x}\right|_{x_j+h/2} = 0$$

ensures each element is insulated from its neighbours.

Diffusion in each element causes exponential decay to an arbitrary constant, say u_j, reflecting the zero eigenvalue.

Centre manifold theory models perturbed dynamical systems: *perturb by funny coupling between elements.*

Parametrise inter-element coupling with γ

$$\begin{aligned} v_j(x_j,t)-v_j(x_{j-1},t) &= \gamma(u_j-u_{j-1})\,, && (1)\\ \text{and}\quad v_j(x_{j+1},t)-v_j(x_j,t) &= \gamma(u_{j+1}-u_j)\,, && (2) \end{aligned}$$

The IBC (2) is the right-hand side IBC of each element and the IBC (1) is the left (same for all problems):

- when $\gamma=0$ these IBCs effectively insulate each element from its neighbours (as LHS $\approx \frac{\partial u}{\partial x}|_{x_j\pm h/2}$); whereas
- when $\gamma=1$ they assert that the field in the jth element analytically extends to the neighbouring grid values.

Centre manifold theory assures:

existence there is an m-dimensional model parametrised by the m grid values u_j

$$u(x,t) = v(\boldsymbol{u}, x, \gamma) \quad \text{such that} \quad \dot{u}_j = g_j(\boldsymbol{u}, \gamma)\,; \qquad (3)$$

relevance the model is exponentially quickly attractive to all nearby solutions of the PDE (no h qualification);

construction it is correct to substitute (3) and solve PDE asymptotically. (routine <blowi_r>)

Include the Dirichlet BC

(1) at the left-hand end $j=1$,

$$v_1(x_1,t)-v_1(x_0,t)=\gamma u_1 \ : \tag{4}$$

- when the coupling parameter $\gamma=0$ this effectively insulates the first element from the conditions at the domain boundary; whereas
- when $\gamma=1$ this reduces to requiring $v_1(x_0,t)=0$.

Computer algebra solves the PDE in elements, using intra-element variable $\xi=(x-x_j)/h$:

$$\begin{aligned} v_1 &= u_1+\tfrac{1}{2}\gamma[u_2\xi+(u_2-2u_1)\xi^2]+\mathcal{O}(\gamma^2)\,, \\ v_2 &= u_2+\tfrac{1}{2}\gamma[(u_3-u_1)\xi+(u_3-2u_2+u_1)\xi^2]+\mathcal{O}(\gamma^2)\,, \end{aligned}$$

and so on.

This looks like simple Lagrange interpolation (when $\gamma=1$).

Actually, leading terms in a sophisticated resolution of physical subgrid structures — good answer to *upscaling*.

The evolution gives the holistic discretisation:

$$
\begin{aligned}
\dot u_1 &= \frac{\gamma}{h^2}u_1(u_2-2u_1) \\
&\quad + \frac{\gamma^2}{12h^2}(-3u_1u_2+3u_2^2-u_2u_3)+\mathcal{O}(\gamma^3)\,, \\
\dot u_2 &= \frac{\gamma}{h^2}u_2(u_3-2u_2+u_1) \\
&\quad + \frac{\gamma^2}{12h^2}(3u_1^2-3u_1u_2+2u_1u_3-3u_2u_3+3u_3^2-u_3u_4) \\
&\quad + \mathcal{O}(\gamma^3)\,,
\end{aligned}
$$

and so on. See modified simple discretisation.

The same bandwidth across the whole domain.

Include boundary forcing $a(t)$

(4) replaced by $$v_1(x_1,t) - v_1(x_0,t) = \gamma(u_1 - a(t))\,. \quad (5)$$

A subgrid field, as if $u_0 = a$ (first line) but:

$$\begin{aligned} v_1 &= u_1 + \tfrac{1}{2}\gamma[(u_2 - a)\xi + (u_2 - 2u_1 + a)\xi^2] \\ &\quad + \frac{\gamma h^2 \dot a}{24 u_1}(\xi+1)\xi(\xi-1)(\xi-2) \\ &\quad + \mathcal{O}(\gamma^2, \ddot a)\,; \end{aligned}$$

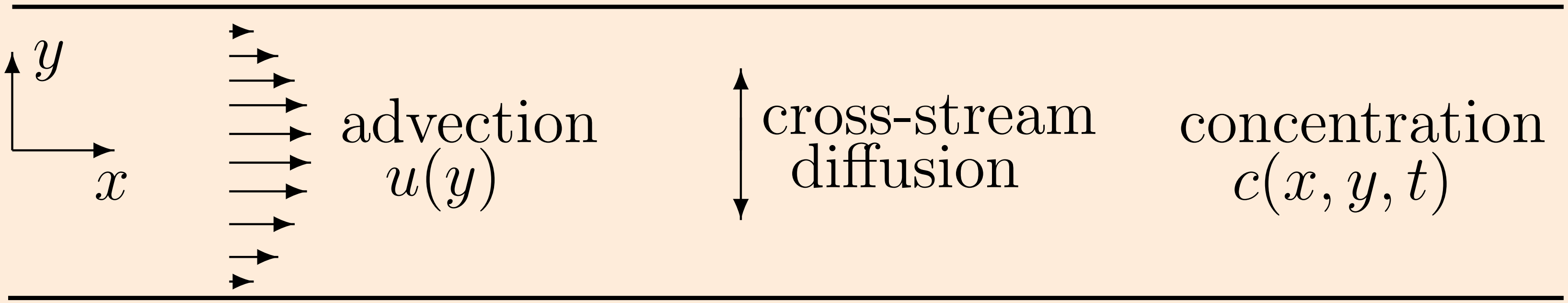
the time derivatives of a represents some of the nonlinear diffusion into the finite sized elements.

The evolution reflects the diffusive time lag:

$$\begin{aligned}\dot u_1 &= \frac{\gamma}{h^2}u_1(u_2-2u_1+a)-\frac{\gamma}{12}\dot a\\ &\quad+\frac{\gamma^2}{12h^2}(a^2-2au_1+2au_2-3u_1u_2+3u_2^2-u_2u_3)\\ &\quad+\frac{\gamma^2\dot a}{720u_1}(25a-6u_1-35u_2)+\mathcal{O}(\gamma^3,\ddot a)\,.\end{aligned}$$

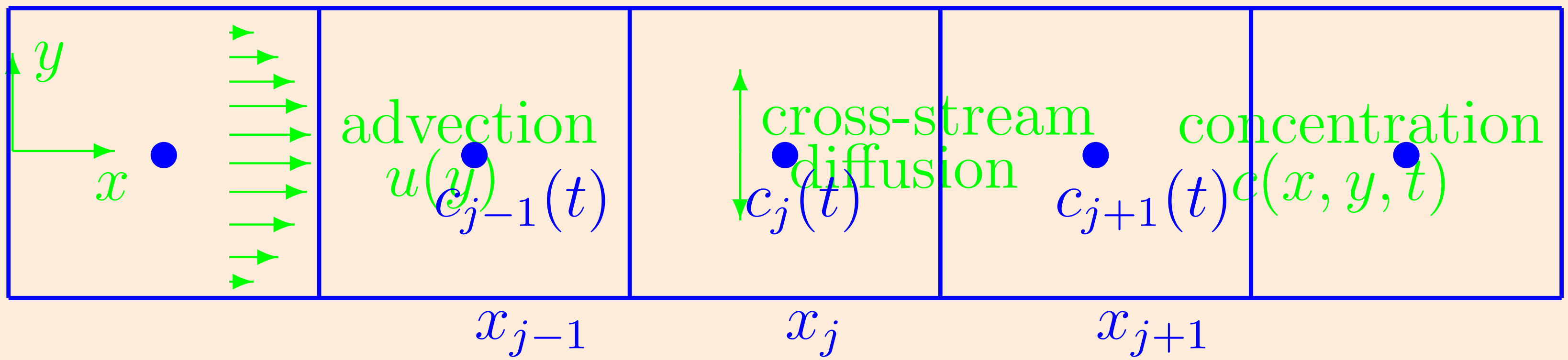
Summary: *This centre manifold approach brings boundary conditions and interior modelling into the one systematic framework.*

2.1 Higher dimension—shear dispersion

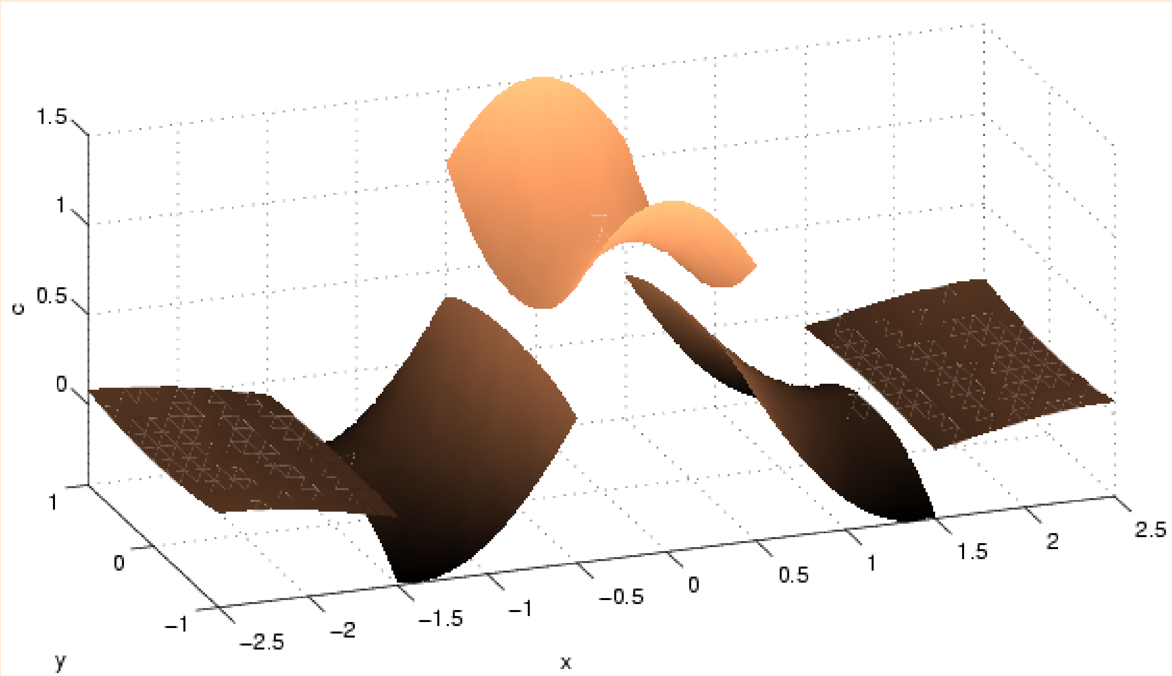


$$\frac{\partial c}{\partial t} = -\mathcal{P}\tfrac{3}{2}(1-y^2)\frac{\partial c}{\partial x} + \boldsymbol{\nabla}\cdot\left[(1-y^2)\boldsymbol{\nabla} c\right] .$$

$$v_j(x_{j+1},y) - v_j(x_j,y) = \gamma\left[v_{j+1}(x_{j+1},y) - v_j(x_j,y)\right] .$$



$$
\begin{aligned}
c &= c_j + \gamma \left[\xi + \frac{\mathcal{P}}{4h} y^2 \right] \mu\delta c_j \\
&\quad + \gamma \left[\frac{1}{2}\xi^2 - \frac{1}{6h^2} y^2 + \frac{\mathcal{P}h}{4}(\xi^3 - \xi) \right] \delta^2 c_j + \mathcal{O}(\gamma^2, \mathcal{P}^2)\,,
\end{aligned}
$$



Evolution: the discretisation is formed by further iteration to γ^2 terms in the element coupling:

$$\begin{aligned}\frac{\partial c_j}{\partial t} &= \frac{2}{3h^2}\left(\gamma\delta^2 - \tfrac{\gamma^2}{12}\delta^4\right)c_j + (\gamma-\gamma^2)\frac{\mathcal{P}^2}{8}\delta^2 c_j + \gamma^2\frac{\mathcal{P}^2}{30h^2}\delta^2 c_j \\ &\quad - \frac{\mathcal{P}}{h}\left(\gamma\mu\delta - \tfrac{\gamma^2}{6}\mu\delta^3\right)c_j - \gamma^2\frac{2\mathcal{P}}{45h^3}\mu\delta^3 c_j \\ &\quad + \gamma^2\left(\frac{2}{135}+\frac{\mathcal{P}^2h^2}{72}-\frac{\mathcal{P}^2h^4}{20}\right)\frac{1}{h^4}\delta^4 c_j + \mathcal{O}(\mathcal{P}^3,\gamma^3)\ : \\ &= x\text{-diffusion} + \text{stabilisation} + \text{shear dispersion} \\ &\quad + \text{advection} + \text{skewness term} \\ &\quad + \text{kurtosis} + \text{h.o.t.}\end{aligned}$$

See that when evaluated at $\gamma = 1$:

- the first term on the right-hand side is an $\mathcal{O}(h^4)$ estimate of the longitudinal diffusion;
- the second term, if truncated to errors $\mathcal{O}(\gamma^2)$, would stablise the discretisation for large advection ($\mathcal{P}$), but here truncated to errors $\mathcal{O}(\gamma^3)$ disappears to leave
- *the third term approximates shear dispersion;*
- whereas the fourth term (the first on the second line above) is an $\mathcal{O}(h^4)$ estimate of the longitudinal advection at mean velocity $\mathcal{P}$;
- the fifth term contributes to the skewness;
- and lastly the sixth term is kurtosis and stabilises.

Summary: *Shear dispersion appears at finite h because we resolve subgrid physical processes.*

3 Continuum models—shear dispersion

Get Taylor model, PDE, as grid size $h \to 0$.

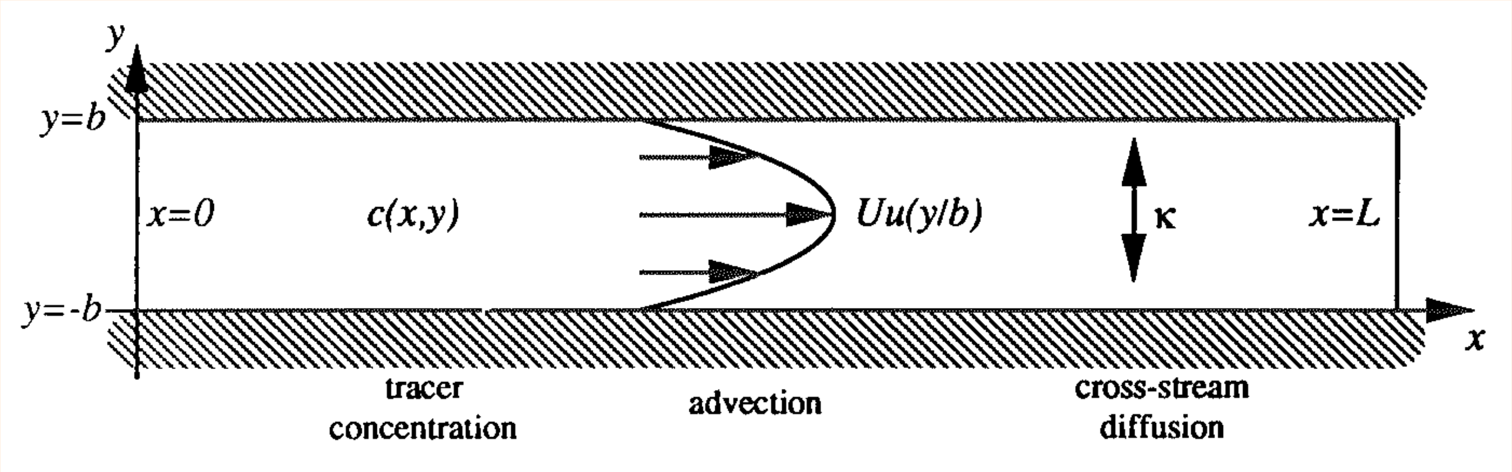
Such spatio-temporal models (PDEs) require BCs:

- dispersion in a river at the the inlet/outlet;
- beams at each end;
- Ginzburg-Landau equations;
- and so on.

BCs provided by two separate arguments; both rely on investigating the *spatial evolution* away from the boundary into the interior (aka Mielke and Iooss).

Both rely on the "initial condition" at the boundary being projected onto the interior model.

3.1 Use an interior model of shear dispersion



$C(x,t)$ is the cross-stream average concentration, concentration field assuming $\partial/\partial x$ is small:

$$c(x,y,t) \;=\; C + \frac{1}{120}\left(-15y^4 + 30y^2 - 7\right)\frac{\partial C}{\partial x} + \cdots\,;$$

where the mean concentration evolves

$$\frac{\partial C}{\partial t} = -\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} + E\frac{\partial^3 C}{\partial x^3} + \cdots\,, \quad D = \frac{2}{105}\,,\ E = \frac{4}{17325}\,.$$

Holds far away from the inlet and outlet.

These infinite sums converge in some sense.

What are the appropriate boundary conditions to be used at inlet $x = 0$, and outlet $x = L$? for various truncations?

Explore the third order model [comment twisty pipe]:

$$\frac{\partial C}{\partial t} = -\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} + E\frac{\partial^3 C}{\partial x^3}\,. \tag{6}$$

Recast in terms of spatial evolution $U = C$, $V = C_x$ and

$W = C_{xx}$:

$$\frac{\partial U}{\partial x} = V\,, \quad \frac{\partial V}{\partial x} = W\,, \quad \frac{\partial W}{\partial x} = \frac{1}{E}U - \frac{D}{E}V + \frac{1}{E}\frac{\partial U}{\partial t}\,.$$

Assume time derivative $\partial/\partial t$ is small perturbation corresponding to slow evolution.

The unperturbed system has *spatial* evolution $\propto e^{\lambda x}$:

- $\lambda_1 = 0$ of the slow evolution in interior;
- $\lambda_2 = 36.42$ of rapid transients near the outlet $x = L$;
- $\lambda_3 = -118.9$ of even more rapid transients near the inflow at $x = 0$.

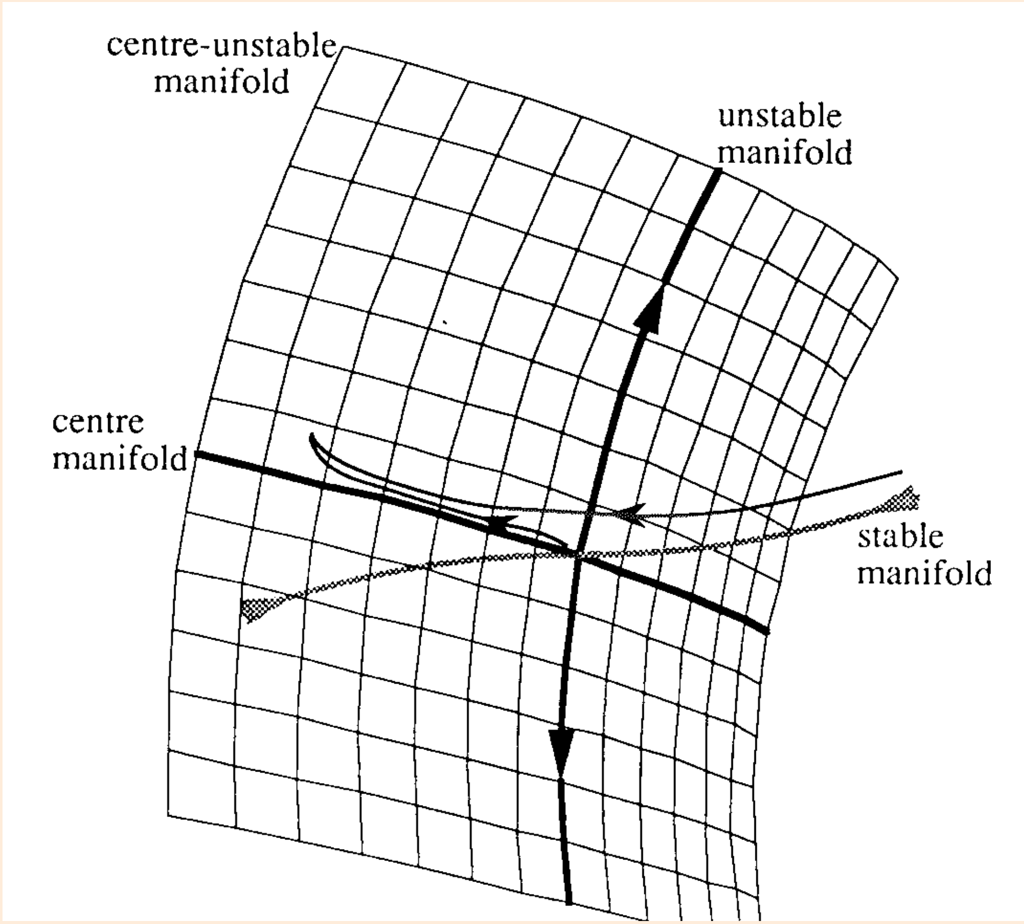
3.2 First of two principles:

the rapid transients must be removed as they are not physical in a slowly varying model.

Here gives two boundary conditions for the model (6):

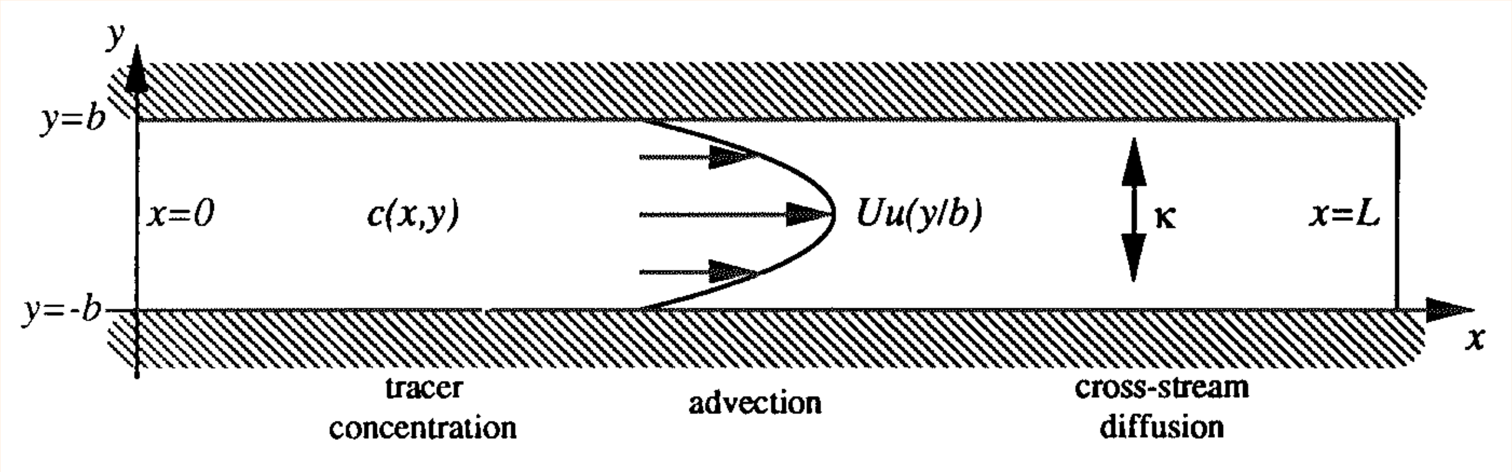
- an inlet to eliminate $e^{36.42\,x}$; and
- an outlet to eliminate $e^{-118.9\,x}$.

Generically require the model to *lie in the centre-unstable manifold of the spatial evolution* away from a boundary into the interior:



centre-unstable manifold has no transients near boundary, and far BCs removes any "unstable dynamics."

3.3 Use the physical dynamics



The concentration $c(x, y, t)$ evolves:

$$\frac{\partial c}{\partial t} = -u(y)\frac{\partial c}{\partial x} + \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \, .$$

Rewrite for spatial evolution with $c' = c_x$:

$$\begin{aligned}\frac{\partial c}{\partial x} &= c' \,, \\ \frac{\partial c'}{\partial x} &= -\frac{\partial^2 c}{\partial y^2} + u(y)c' + \frac{\partial c}{\partial t} \,,\end{aligned}$$

Focus on slow evolving solutions for which $\partial/\partial t \approx 0$; the *spatial evolution* has eigenvalues

- one $\lambda = 0$ of the slowly varying shear dispersion model
$$\frac{\partial C}{\partial x} = -\frac{\partial C}{\partial t} + \frac{2}{105}\frac{\partial^2 C}{\partial t^2} - \frac{116}{121275}\frac{\partial^3 C}{\partial t^3} + \cdots \,;$$
- $\lambda = -3.414\,, -12.25\,, \ldots$ of rapid transients;
- and infinitely many positive eigenvalue transients.

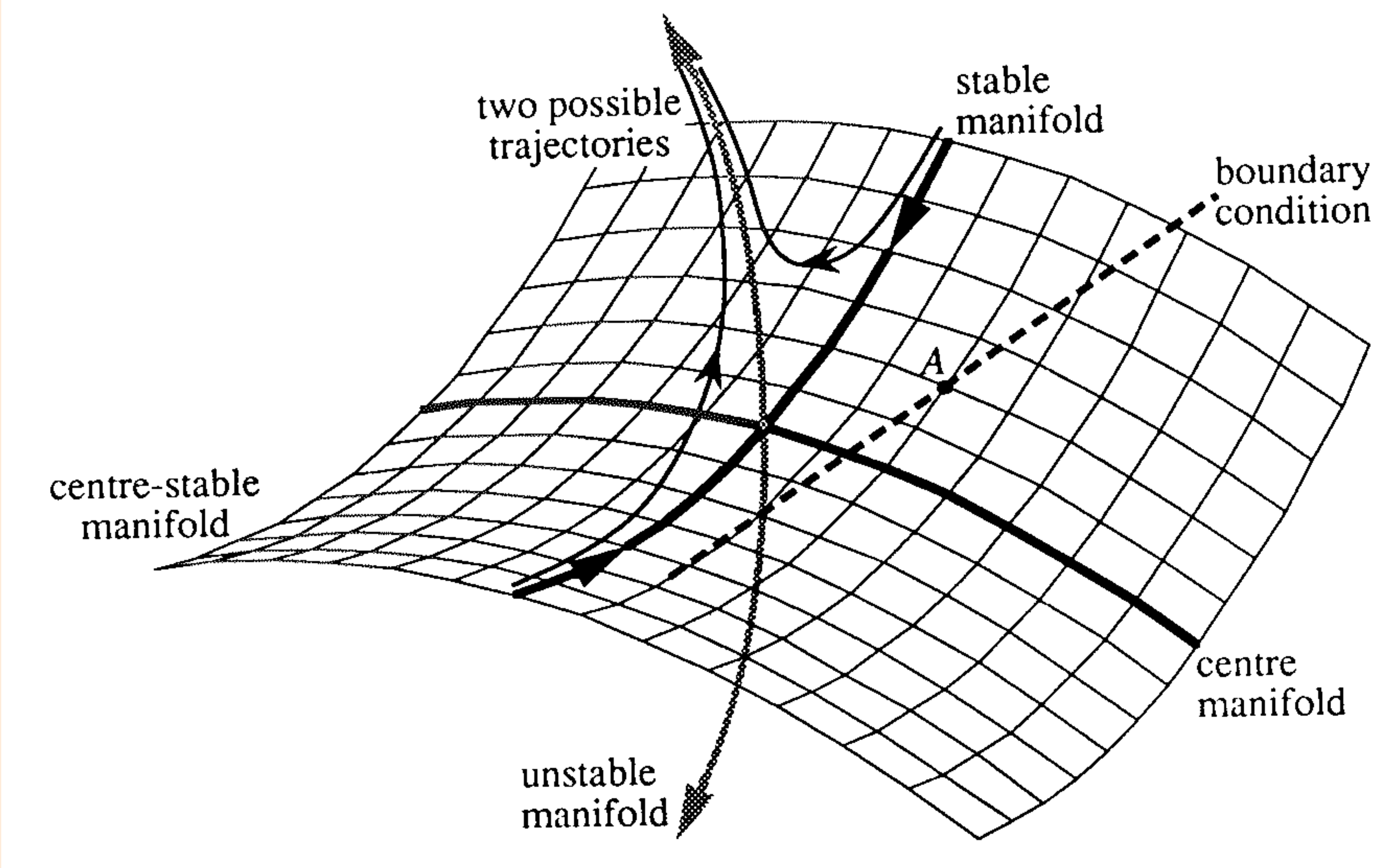
At the inlet there cannot be any component of the last positive eigenvalue modes as these would blow up in the interior.

However, the physical inlet condition typically will have spatially decaying transients. For example, a pipe may be discharging waste into the side of the channel at $x = 0$.

The effective inlet condition for the cross-stream average concentration $C(0, t)$ is the value after these transients have died out.

Use the adjoint eigenmode of $\lambda = 0$ to project the physical inlet condition to a boundary condition for the model.

Generically, the second principle of reality:



1. the physical fields must lie in the centre-stable manifold of the spatial evolution away from the boundary;
2. the physical boundary conditions intersect a set of states on the centre-stable manifold;
3. “initial condition” arguments project these states onto the slow manifold of the interior model along isochrons; <isochron>
4. the codimension of the projected set is effectively the number of boundary conditions for the model.

At the outlet of the channel the codimension is zero, so there is *not* another boundary condition for the model.

The transients in negative x direction are the complete modes of the positive eigenvalues.

These fit any physical outlet condition, exponentially quickly in space.

The physical outlet places no restriction on the model (6).

Great because we already have three BC.

4 Conclusion

Two different scenarios:

- direct modelling of divided and reglued space naturally adapts to physical boundaries at finite grid size by resolving subgrid fields;
- “spatial dynamics” provides a completely different mechanism for resolving the influence of “transients” we otherwise know as boundary layers.

Moreover, ...

State space arguments derive accurate and reliable low-dimensional models of spatio-temporal dynamics from a detailed description:

- the signature of the model is derived from linearisation;
- the modelling is systematically refined;
- produces appropriate boundary conditions.

Lastly, there also exists a third approach: *it is completely unclear to me as to whether these disparate approaches produce equivalent boundary conditions!*