Chaotic Advection in Thin Films?

Jean-Luc Thiffeault and Khalid Kamhawi

Department of Mathematics
Imperial College London

FACM, NJIT, 16 May 2006

Introduction

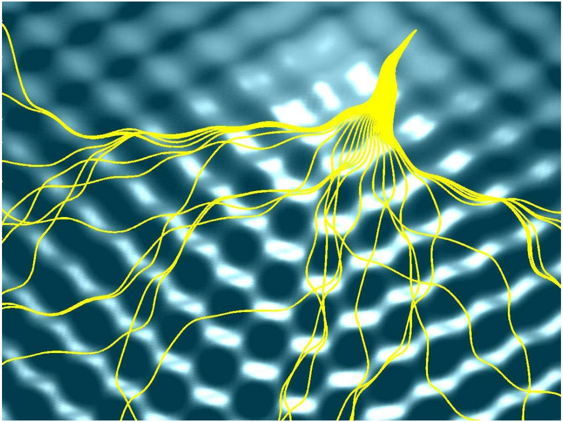
- A thin layer of fluid flowing down an inclined substrate.
- Reduce to two-dimensional problem by asymptotic expansion: PDE for the height field.
- But the velocity field is still three-dimensional, with a nontrivial vertical component.
- Steady three-dimensional flows can exhibit chaotic trajectories.
- This leads to fluid particles rapidly decorrelating: good for mixing.
- Can suitable substrate shapes lead to good horizontal mixing?

Strategy

- Thin-layer expansion in the direction normal to the substrate.
- Similar derivation to [Roy, Roberts, and Simpson, *JFM* **454**, 235 (2002)].
- For simplicity, assume steady flow.
- Use non-orthogonal coordinates, since globally orthogonal coordinates do not usually exist.
- Correct velocity field to satisfy kinematic constraints — this is crucial for particle advection.
- Integrate trajectories and make Poincaré sections in a spatially periodic domain.

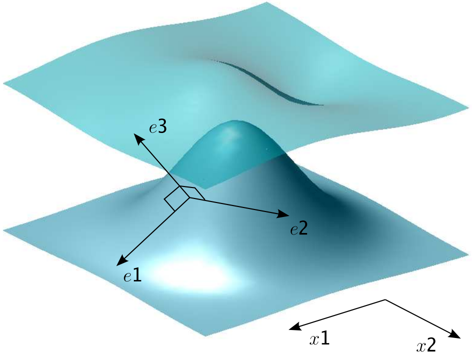
Aside: Inviscid Theory

Inertia is great for chaos. . .



. . . but particle trajectories (characteristics) cross all over the place.
Fix as Sam Howison did yesterday?

Coordinate System



Surface $y = \eta(x^1, x^2)$

Substrate $y = 0$
at position $\mathbf{X}(x^1, x^2)$

$$\mathbf{r}(x^1, x^2, y) = \mathbf{X}(x^1, x^2) + y\,\hat{\mathbf{e}}_3(x^1, x^2)$$

$$\mathbf{e}_\alpha = \frac{\partial \mathbf{X}}{\partial x^\alpha} = \partial_\alpha \mathbf{X}\,; \qquad \hat{\mathbf{e}}_3 = (\mathbf{e}_1 \times \mathbf{e}_2)/\left\|\mathbf{e}_1 \times \mathbf{e}_2\right\|$$

Coordinate Vectors in the Bulk

Vectors corresponding to coordinates in the fluid:

$$\tilde{\mathbf{e}}_\alpha = \partial_\alpha \mathbf{r} = \mathbf{e}_\alpha - y\,\mathbb{K}_\alpha{}^\beta\,\mathbf{e}_\beta\,, \qquad \tilde{\mathbf{e}}_3 = \mathbf{e}_3 = \hat{\mathbf{e}}_3 = \frac{\partial \mathbf{r}}{\partial y}\,,$$

- Summation of repeated indices;
- Greek indices always take the value 1 or 2 (never 3);
- Roman indices always take the value 1, 2, or 3;
- Tilde quantities are evaluated in the 'bulk' (away from the substrate), and thus depend on y.

Curvature tensor $\mathbb{K}_\alpha{}^\beta$ defined by

$$\partial_\alpha \hat{\mathbf{e}}_3 = -\mathbb{K}_\alpha{}^\beta\,\mathbf{e}_\beta\,,$$

Note that the $\mathbf{e}_\alpha$ are not necessarily orthogonal or normalised.

Metric Tensor

To express the length of vectors in the (x^1, x^2, y) coordinates, we need the metric tensor $\tilde{\mathfrak{g}}_{\alpha\beta}$

$$\tilde{\mathfrak{g}}_{ij} = \tilde{\mathbf{e}}_i \cdot \tilde{\mathbf{e}}_j = \begin{pmatrix} \widetilde{\mathbb{G}}_{\alpha\beta} & 0 \\ 0 & 1 \end{pmatrix}$$

where

$$\widetilde{\mathbb{G}}_{\alpha\beta} := \tilde{\mathbf{e}}_\alpha \cdot \tilde{\mathbf{e}}_\beta = \mathbb{G}_{\alpha\beta} - 2y\, \mathbb{K}_{\alpha\beta} + y^2\, \mathbb{K}_\alpha{}^\gamma\, \mathbb{K}_{\gamma\beta}\,,$$
$$\mathbb{G}_{\alpha\beta} := \mathbf{e}_\alpha \cdot \mathbf{e}_\beta\,.$$

The full metric $\tilde{\mathfrak{g}}_{ij}$ is block-diagonal. The 2×2 metric $\mathbb{G}_{\alpha\beta}$ is the surface metric, and $\widetilde{\mathbb{G}}_{\alpha\beta}$ is its extension into the bulk of the fluid. We have used the surface metric to lower an index on $\mathbb{K}$:

$$\mathbb{K}_{\alpha\beta} = \mathbb{G}_{\alpha\gamma}\mathbb{K}_\beta{}^\gamma$$

The Dilatation of the Coordinates

A crucial quantity is the determinant of the metric,

$$\tilde{w} = \left(\det \widetilde{\mathbb{G}}_{\alpha\beta}\right)^{1/2} = \tilde{\omega}\, w, \qquad w = \left(\det \mathbb{G}_{\alpha\beta}\right)^{1/2},$$

where

$$\tilde{\omega} = 1 - \kappa\, y + \mathcal{G}\, y^2\,,$$

and

$$\kappa = \mathbb{K}_{\alpha}{}^{\alpha} \qquad \text{mean curvature;}$$

$$\mathcal{G} = \det \mathbb{K}_{\alpha}{}^{\beta} \qquad \text{Gaussian curvature.}$$

The volume element is given by by $\tilde{\omega}\, w\, dx^1 dx^2 dy$.
If $\tilde{\omega}$ becomes negative, then substrate normals cross within the fluid and the coordinate system becomes invalid. OK as long as

$$0 \le y < \{\max(k_1, k_2, 0^+)\}^{-1}\,, \qquad k_{1,2} := \tfrac{1}{2}\left(\kappa \pm \sqrt{\kappa^2 - 4\mathcal{G}}\right),$$

where k_1 and k_2 are the principal curvatures.

Notation

There are three types of quantities in our development:

1. Quantities with a **tilde** (e.g., $\tilde{\mathbf{e}}_\alpha$ and $\tilde{w}$) are evaluated between the substrate and the free surface and are functions of (x^1, x^2, y).
2. Quantities with an **overbar** (e.g., $\bar{\mathbf{e}}_\alpha$ and $\bar{w}$) are evaluated on the free surface $y = \eta(x^1, x^2)$ and are functions of (x^1, x^2).
3. **'Bare-headed'** quantities (e.g., $\mathbf{e}_\alpha$ and w) are evaluated on the substrate $y = 0$ and are functions of (x^1, x^2), or they are quantities that do not depend on y at all (e.g., $\hat{\mathbf{e}}_3$).

Mass Conservation

We introduce a steady velocity field

$$\mathbf{u} = \tilde{u}^{\alpha}\,\tilde{\mathbf{e}}_{\alpha} + \tilde{v}\,\hat{\mathbf{e}}_3\,.$$

Mass conservation is imposed via the divergence-free condition, $\nabla \cdot \mathbf{u} = 0$; in terms of our coordinates,

$$\partial_{\alpha}\left(\tilde{w}\,\tilde{u}^{\alpha}\right) + \frac{\partial}{\partial y}\left(\tilde{w}\,\tilde{v}\right) = 0\,.$$

We integrate this from 0 to η and use the no-throughflow condition $\tilde{v}(x^1, x^2) = 0$ to get

$$\bar{w}\,\bar{v} = -\int_0^{\eta} \partial_{\alpha}\left(\tilde{w}\,\tilde{u}^{\alpha}\right)\,\mathrm{d}y = \bar{w}\,\bar{u}^{\alpha}\partial_{\alpha}\eta - \partial_{\alpha}\int_0^{\eta}\left(\tilde{w}\,\tilde{u}^{\alpha}\right)\,\mathrm{d}y.$$

Mass Conservation (cont'd)

Now we use the kinematic boundary condition at the top surface,

$$\bar{u}^\alpha\,\partial_\alpha \eta = \bar{v},$$

to find

$$\partial_\alpha\left(w\,\bar{q}^\alpha\right) = 0,$$

where the flux vector is

$$\tilde{q}^\alpha(x^1, x^2, y) := \int_0^y \tilde{\omega}\,\tilde{u}^\alpha dy\,, \qquad \bar{q}^\alpha(x^1, x^2) = \tilde{q}^\alpha(x^1, x^2, \eta).$$

If we divide through by w, we recognise the covariant divergence,

$$\nabla_\alpha \bar{q}^\alpha = 0.$$

Note that there are no assumptions on the thinness of the layer: everything is exact.

Dynamical Equations

We now assume $\mathbf{u}$ satisfies the Stokes equation,

$$\Delta \mathbf{u} = \nabla p - \hat{\mathbf{g}},$$

where p is the pressure and $\hat{\mathbf{g}}$ is a unit vector in the direction of gravity. The velocity satisfies the boundary conditions

$$\begin{aligned} \mathbf{u} &= 0 && \text{at } y = 0 && \text{no-slip at substrate} \\ \mathbf{t}_\alpha \cdot \tau \cdot \hat{\mathbf{n}} &= 0 && \text{at } y = \eta && \text{tangential stresses at free surface} \\ -p + \hat{\mathbf{n}} \cdot \tau \cdot \hat{\mathbf{n}} &= \sigma \kappa_{\text{surf}} && \text{at } y = \eta && \text{normal stress at free surface} \end{aligned}$$

where

$$\tau := \nabla \mathbf{u} + (\nabla \mathbf{u})^T$$

is the deviatoric stress, $\hat{\mathbf{n}}$ is the unit normal to the surface, $\mathbf{t}_\alpha$ are tangents to the surface, and κ_{surf} is the mean curvature of the surface. All quantities are dimensionless.

Small-parameter Rescaling

The time has come to make the layer thin: we do this by assuming that horizontal scales vary slowly:

$$x^\alpha = \varepsilon^{-1}\, x^{\alpha *}, \quad \tilde{v} = \varepsilon\, \tilde{v}^*, \quad p = \varepsilon^{-1}\, p^*, \quad \sigma = \varepsilon^{-2}\, \sigma^*.$$

Everything else is of order unity, including vertical scales. We immediately drop the * superscripts, and expand the fields as

$$\begin{aligned} \tilde{u}^\alpha &= \tilde{u}^\alpha_{(0)} + \varepsilon\, \tilde{u}^\alpha_{(1)} + \dots, \\ \tilde{p} &= \tilde{p}_{(0)} + \varepsilon\, \tilde{p}_{(1)} + \dots. \end{aligned}$$

Note that we leave $\tilde{v}$ unexpanded (more on this later).

Order ε^0

At order ε^0, the velocity field and pressure satisfy

$$\frac{\partial^2 \tilde{u}^\alpha_{(0)}}{\partial y^2} = \partial^\alpha \tilde{p}_{(0)} - \hat{g}^\alpha_{\mathrm{s}}\,, \qquad \frac{\partial \tilde{p}_{(0)}}{\partial y} = 0\,,$$

where $\partial^\alpha = \mathbb{G}^{\alpha\beta}\,\partial_\beta$. These are readily integrated to give

$$\tilde{u}^\alpha_{(0)} = -\tfrac{1}{2}\left(\hat{g}^\alpha_{\mathrm{s}} + \sigma\,\partial^\alpha\kappa\right)\,y(y-2\eta), \qquad \tilde{p}_{(0)} = -\sigma\kappa,$$

where the boundary conditions have been applied.

Order ε^1

At order ε,

$$\frac{\partial^2 \tilde{u}^{\alpha}_{(1)}}{\partial y^2} = \left(\kappa \delta_{\beta}{}^{\alpha} + 2\,\mathbb{K}_{\beta}{}^{\alpha}\right) \frac{\partial \tilde{u}^{\beta}_{(0)}}{\partial y} + \partial^{\alpha} \tilde{p}_{(1)} + 2y\,\mathbb{K}_{\beta}{}^{\alpha} \partial^{\beta} \tilde{p}_{(0)} - y\,\hat{g}^{\beta}_{\mathrm{s}}\,\mathbb{K}_{\beta}{}^{\alpha}\,,$$

with solution

$$\tilde{u}^{\alpha}_{(1)} = A^{\alpha}_{(1)} y\left(y - 2\eta\right) + B^{\alpha}_{(1)} y\left(y^2 - 3\eta^2\right)$$

where the coefficients $A^{\alpha}_{(1)}$ and $B^{\alpha}_{(1)}$ involve the substrate curvature tensor and gradients of the mean curvature.
In fact, the ε^0 solution can be incorporated to the coefficient A, to give

$$\tilde{u}^{\alpha} = A^{\alpha} y\left(y - 2\eta\right) + B^{\alpha} y\left(y^2 - 3\eta^2\right).$$

The Mass Flux

The horizontal velocity field is sufficient to find the mass flux,

$$\bar{q}^\alpha = \int_0^\eta \tilde{\omega}\,\tilde{u}^\alpha dy = \int_0^\eta (1 - \varepsilon\,\kappa\,y)\tilde{u}^\alpha\,dy + \mathcal{O}\big(\varepsilon^2\big)\,,$$
$$= \bar{q}^\alpha_{\rm grav} + \bar{q}^\alpha_{\rm surf}\,,$$

$$\bar{q}^\alpha_{\rm grav} = \tfrac{1}{3}\eta^3\left\{\hat{g}^\alpha_{\rm s} - \varepsilon\,\hat{g}^\beta_{\rm s}\left(\kappa\,\delta_\beta{}^\alpha + \tfrac{1}{2}\,\mathbb{K}_\beta{}^\alpha\right)\eta + \varepsilon\,\hat{g}_y\,\partial^\alpha\eta\right\}$$
$$+\varepsilon^2\frac{1}{120}\,\eta^4\kappa\left\{\eta\,\hat{g}^\beta_{\rm s}\,(9\kappa\,\delta_\beta{}^\alpha + 11\,\mathbb{K}_\beta{}^\alpha) - 25\,\hat{g}_y\,\partial^\alpha\eta\right\} + \mathcal{O}\big(\varepsilon^2\big),$$

$$\bar{q}^\alpha_{\rm surf} = \tfrac{1}{3}\sigma\eta^3\left\{\partial^\alpha\kappa_{\rm surf} - \varepsilon\,\eta\,\kappa\,\partial^\alpha\kappa + \tfrac{1}{2}\varepsilon\,\eta\,\mathbb{K}_\beta{}^\alpha\,\partial^\beta\kappa\right\}$$
$$+\varepsilon^2\frac{1}{120}\,\sigma\,\eta^4\kappa\left\{9\eta\,\kappa\,\partial^\alpha\kappa - 14\,\eta\mathbb{K}_\beta{}^\alpha\partial^\beta\kappa - 25\,\partial^\alpha(\kappa_2\eta + \Delta\eta)\right\} + \mathcal{O}\big(\varepsilon^2\big),$$

Note that we've kept some second-order terms but not others. The above fluxes are only asymptotic to order ε^1, but they preserve the free-surface kinematic BC to all orders...

The Vertical Velocity

The vertical velocity is obtained from mass conservation:

$$\tilde{v} = -\frac{1}{1-\varepsilon\kappa y}\int_0^y \partial_\alpha\left(\left(1-\varepsilon\kappa y\right)\tilde{u}^\alpha\right)\,dy\,, \quad \text{not expanded in } \varepsilon.$$

Mass conservation follows from using this form for $\tilde{v}$, and the free-surface kinematic boundary condition is satisfied exactly if the second-order terms are included in the flux.

The exact kinematic constraints are crucial for particle advection:

- Mass preservation prevents the existence of attractors in the flow where particles bunch up.
- The kinematic boundary condition prevents particles escaping from the top surface of the flow.

These are only exact to the extent that $\nabla_\alpha \bar{q}^\alpha = 0$ is satisfied numerically, but this is a much smaller error than ε^2.

The Shape of the Substrate

The shape of the bottom substrate is given by the vector $\mathbf{X}(x^1, x^2)$. The generality of the formulation allows us to choose (x^1, x^2) as cylindrical (or any other) coordinates, which could be used to describe a 'bumpy fibre.' However, we stick to Cartesian and write

$$\mathbf{X}(x^1, x^2) = (x^1 \ x^2 \ f(x^1, x^2))^T,$$

which rules out a multivalued substrate (no overhangs). $f(x^1, x^2)$ gives the vertical height of the substrate at (x^1, x^2).

We assume the substrate is periodic in both directions.

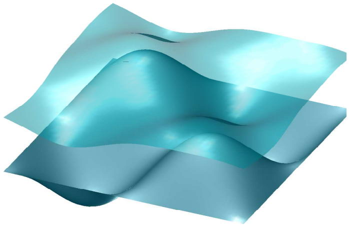
The flow is driven by the tilt θ of the gravity vector with respect to the substrate:

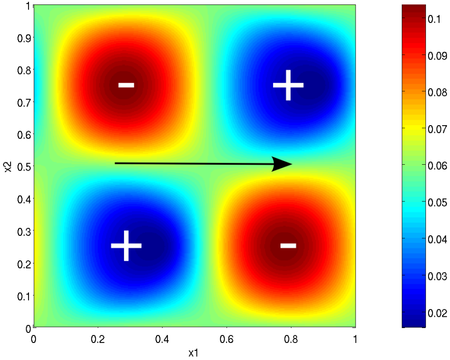
$$\hat{\mathbf{g}} = (\sin\theta\cos\phi \quad \sin\theta\sin\phi \quad -\cos\theta)^T$$

Numerical Solution

We now solve $\nabla_\alpha \bar{q}^\alpha = 0$ for the height field $\eta(x^1, x^2)$. The pictures below are for

$$f(x^1, x^2) = f_0 \sin(2\pi x^1) \sin(2\pi x^2).$$





Parameters: $f_0 = 0.05$, $\varepsilon = 0.06$, $\theta = 0.1$, $\phi = 0$, $\sigma = 0$.

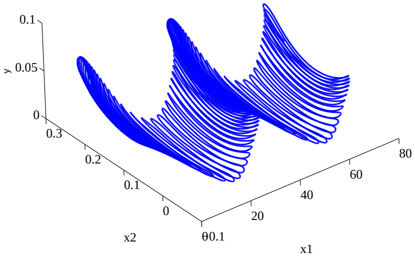
Numerical Error in Kinematic BC

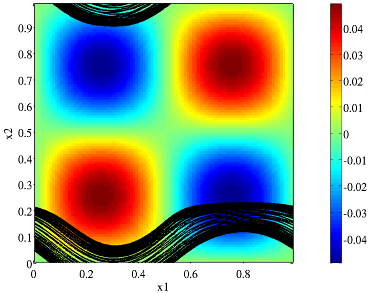
For a numerical resolution of 100×100,

	Uncorrected	Corrected
Kinematic BC error	4×10^{-4}	2×10^{-9}
Incompressibility error	4×10^{-3}	9×10^{-7}

The factor of 10^4–10^5 improvement makes a huge difference when doing particle advection: it means that particles can skirt the surface without escaping.

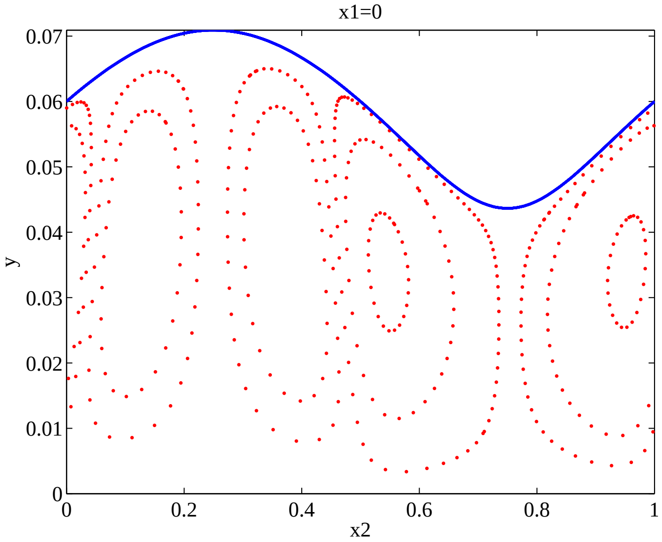
A Typical Trajectory





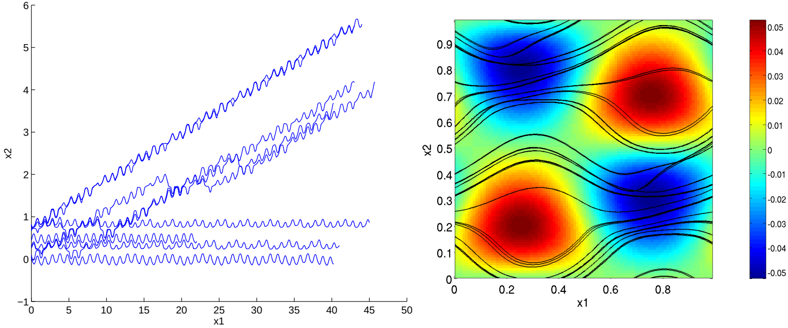
- The particle explores the top and bottom of the layer.
- It is confined in a narrow region in x^2.

Poincaré Section



Breaking the Symmetry

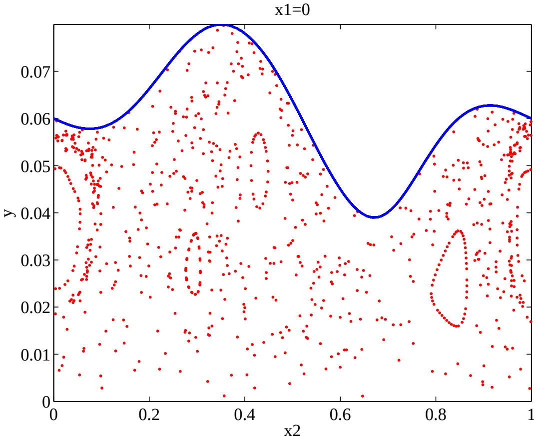
$$f(x^1, x^2) = f_0 \left\{ \sin(2\pi x^1) \sin(2\pi x^2) + \delta \sin(4\pi x^2) \right\}, \quad \delta = 0.2$$



- Two types of trajectories: straight and diagonal.
- Explore a wide range in x^2.
- The diagonal trajectories are chaotic: 'jump' between channels.

Chaotic Poincaré Section

The mixed regular–chaotic phase space is evident in the section:



Conclusions

- Relate substrate properties (curvature tensor) to chaotic features.
- Applications? Coating flows?
- Experiments
- Time-dependence: induce chaotic mixing by vibrating the substrate or sending waves through it.
- Effect of surfactants, surface tension, Marangoni stresses. . .