NEPTUNE UQ - Coupled 1D turbulence and diffusion, November 2022
Ed Threlfall

1 Abstract

This document outlines two proxyapps representing a 1D turbulence proxy (represented by the well-known Lorenz model) coupled to a 1D time-dependent diffusion problem.

2 Motivation

Coupled turbulent heat transfer and diffusion is relevant for the Smallab experiment, in which a turbulent fluid tank is coupled to diffusion through the solid tank walls.

There is not yet very much code in NEPTUNE that can be used to explore coupled models.

This work provides a one-way coupled model and also an initial attempt at a fully-coupled implementation in which the diffusion model affects the turbulent model.

The implementations are small C++ codes which execute in very little time on an ordinary laptop.

3 Work

3.1 Coupled models

An interesting coupled system is one-way coupling between a turbulent fluid model of heat transfer and ordinary isotropic heat conduction - needs to be done in time-domain because of the non-time-stationary quasi-steady state of the fluid model. This will be possible in *Nektar++* once coupling via boundary data is implemented. A 1D practice case is to use the Nusselt number output of the Lorenz model (which has 3 input parameters, Pr, Ra, and one other) as boundary data (Neumann) for a 1D time-dependent diffusion problem.

The turbulent model is the *Lorenz model*, which is derived from a 2D model of Rayleigh-Bénard convection,

$$\begin{aligned} \dot{x} &= \sigma(y-x), \\ \dot{y} &= x(\rho-z)-y, \\ \dot{z} &= xy-\beta z. \end{aligned} \tag{1}$$

The parameters ρ, σ, β are respectively the Rayleigh number, the Prandtl number, and the coupling strength. In the original model, the Rayleigh number is $\rho \equiv \frac{\Delta T - \Delta T_c}{\Delta T_c}$ i.e. the temperature difference applied across the vertical direction of the convecting cavity. The Nusselt number for this model, representing the heat flux out, is $Nu = 1 + \frac{2z}{\rho}$ - this has a minimum value of 1 which corresponds to the conducting limit.

The parameters used for this study were the canonical choices $\rho = 28$, $\sigma = 10$, $\beta = \frac{8}{3}$, which gives an unsteady time-evolution.

The diffusion model is

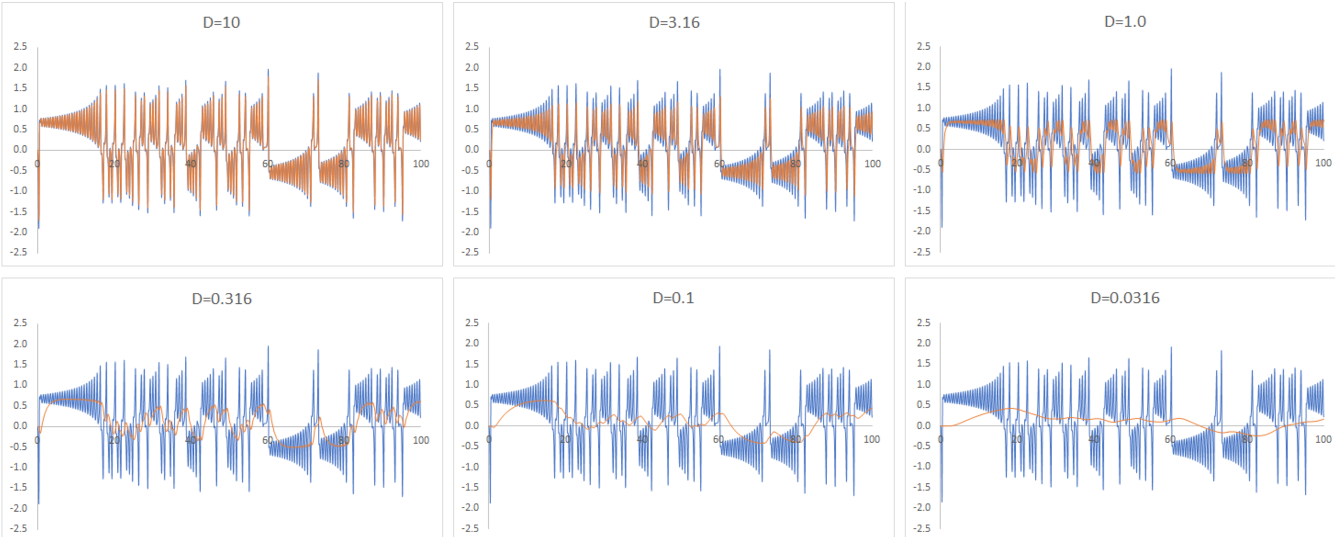

Figure 1: Output time series from the diffusion model, showing heat flux into the left-hand-side (blue) and heat flux out of the right-hand-side (orange), for various values of diffusivity D. In the limit of large D, the output matches the input. Note that the time-averaged averaged heat fluxes in and out are the same. (Axes: horizontal is time, vertical is heat flux.)

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}. \tag{3}$$

This model will take the heat flux on the left-hand-side of the interval $[0, 1]$ as a Neumann boundary condition (note definition of heat flux as $F = -D\frac{dT}{dx}$ where D is the diffusivity). The boundary condition at the right-hand-side of the diffusing interval is homogeneous Dirichlet, $T = 0$.

Both models can obviously be run without HPC, and model outputs easily checked against literature (see [3] for the Lorenz model).

3.2 One-way-coupled model

The code described here can be found at [1].

In this model the Nusselt number (or other output) is used as the input to a 1D time-dependent diffusion problem. Note in this case the y time series outputs were used, as these exhibit greater variability than the always-positive Nusselt number time series.

It can be seen (Fig.1) that large values of the diffusivity D preserve the input series, whereas increased values of D lead to a damping of the heat flux response as well as a low-pass filtering effect.

One minor point here is that the gradient used for the Neumann condition in the diffusion problem is the positive Nusselt number; physically the negative gradient should be used and it should be scaled from a heat flux to a temperature gradient - these considerations are, however, unimportant for the linear, non-back-reacted diffusion case. (This issue is fixed in the model described in the next section.)

It is easily possible to replace the Lorenz ODE system with another ODE for testing purposes (e.g. a linear oscillator) - just modify the function `Lorenz::EvaluateTimeDerivs`.

The ‘phase diagram’ of the Lorenz model alone is easily investigated [3] with small modifications to the code. Fig.2 shows outputs of 40,000 model runs and each was generated in c.1min on a laptop.

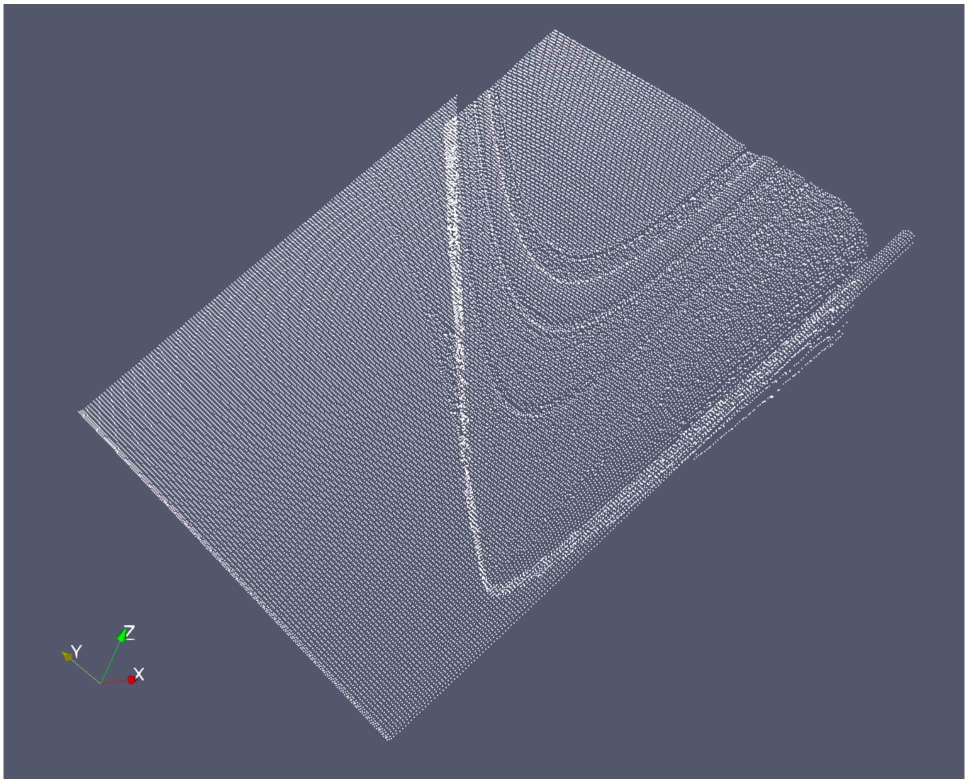

Figure 2: 'Phase diagram' of the Lorenz model: the z-axis is the averaged value of $z(t)$, the x-axis is the Rayleigh number in the range $[0, 100]$ and the y-axis is the Prandtl number in $[0, 100]$. For much better plots, see [3].

Questions:

- Can the input parameters to the Lorenz model (concentrate on Rayleigh and Prandtl numbers) be inferred from one (or more) of the time-series outputs?
- Can the above inference be applied after some diffusion has taken place?
- Does state-space reconstruction still work for the Lorenz model after some diffusion has taken place?

3.3 Two-way coupled model

The code described here can be found at [2].

The diffusion problem can be made to back-react on the Lorenz model by allowing the temperature T_L at the entry point to the diffusive region to determine the Rayleigh number ρ in the Lorenz model. The connection needs to be made via some function that avoids pathological behaviours; reasonable properties would seem to be that ρ decreases monotonically with increasing T_L and that ρ cannot become negative. In practice, a function that ensures $\rho \geq 1$ appears to work better than one that is allowed to decrease to zero (note that $\rho = 1$ does correspond to a fixed point with $Nu = 1$ representing the conduction-only heat transfer regime). The empirical function $\rho = 1 + 27e^{-T_L}$ was chosen; for the initial condition $T_L = 0$ this represents the same choice of parameters as used in the previous section. (Note that, with this function and positive temperatures, the Rayleigh number has a maximum value of 28.) *It seems likely that there are more sensible choices of this function.*

The parameters σ and β take the same fixed values as in the previous section.

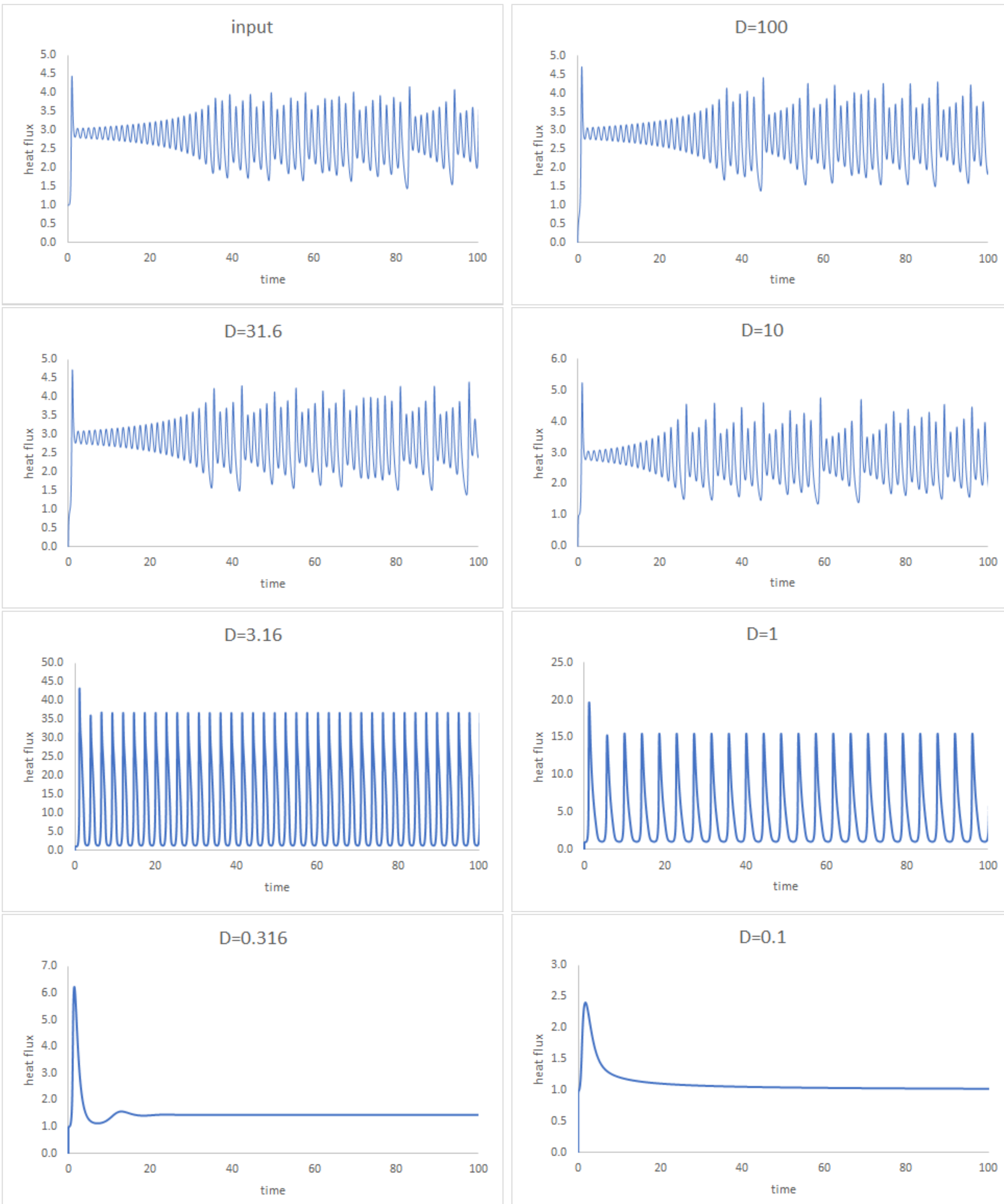

Figure 3: Time series heat flux *inputs* of the coupled Lorenz and diffusion model for various values of the diffusivity D, i.e. the heat flux entering the diffusive region from the turbulent model, which is affected by the back-reaction of the diffusion problem on the Lorenz series in the way explained in the main text.

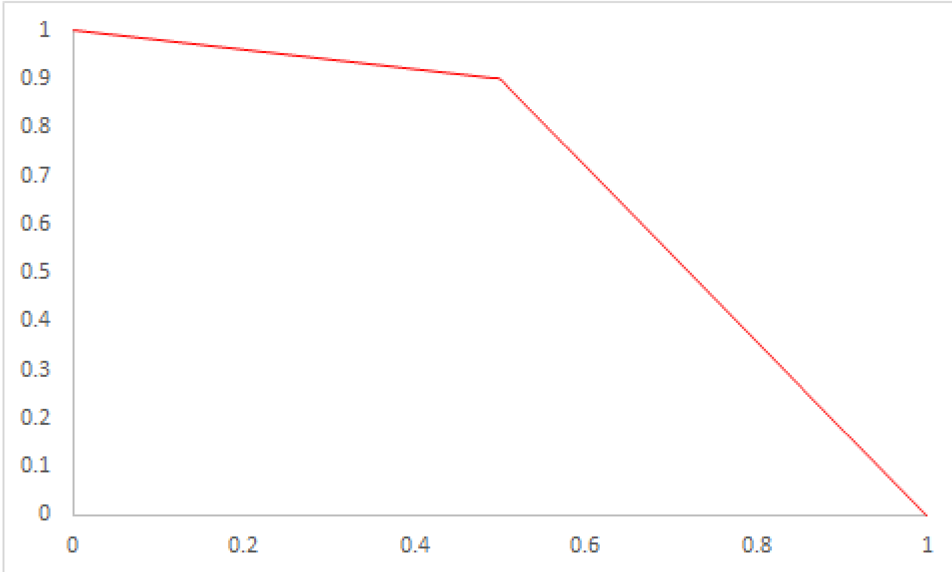

Figure 4: PROBLEM. Steady-state temperature profile across a block consisting of two different materials in regions $[0, 0.5]$ and [0.5,1]. *Which region is the better conductor of heat?*

Outputs can be seen in Fig.3; these are the time series for the heat flux into the diffusive region. It can be seen that for large values of D preserves well the no-coupling input heat flux (the diffusion is rapid, therefore the temperature is near-uniform across the diffusive region). Small values of D result in a 'turning off' of the turbulence, which physically is supposed to represent the fact that insulating the turbulent region reduces the temperature gradient across it (the fluid is hotter but remember that turbulence is driven by temperature *gradients*) - one sees that the turbulent time series is brought into a quiescent state and the heat flux (Nusselt number) tends to unity, which is the minimum possible rate of heat transfer in this model, corresponding to pure conduction. In between these regimes there is an oscillatory regime in which, strangely, the average heat flux is enhanced over the turbulent case - it is expected that this non-monotonicity reflects the non-physical nature of the model, either from the extrapolation of the Lorenz single-mode approximation beyond its region of validity or from the coupling function that was chosen empirically.

4 General questions

- Which parts of the UCL task work are these models useful for?

References

[1] https://github.com/ethrelfall/Coupled-heat-transport.

[2] https://github.com/ethrelfall/Two-way-coupled-heat-transport.

[3] H.R. Dullin, S. Schmidt, P.H. Richter, and S.K. Grossmann, *Extended phase diagram of the Lorenz model*, International Journal of Bifurcation and Chaos Vol.17 No.09, pp3013-3033 (2007).