Contents

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Good approximations often lead to better ones.

Mathematical Methods in Science
George Pòlya, 1977

Chapter 4

Calculation and modelling of subgrid tendencies

TODO: introductory paragraph: why am I doing this?

4.1 Calculation of subgrid tendencies

The method used to calculate the subgrid tendencies is described below and illustrated in the form of a flowchart in Figure 4.1.

1. The fine model was integrated for [TODO:] time units. Every 3 time units, the model state was saved, and then saved again one time step later. This resulted in a dataset of [TODO:] pairs of snapshots separated by 3 time units. An interval of 3 time units was chosen as it was the approximate decorrelation time of the model state (see Appendix A.5); using a shorter interval would mean saving redundant information.

2. The first snapshot in each pair was subtracted from the second snapshot and the difference divided by the time step, giving the *fine tendency* (i.e., the time derivative of the fine model state).

3. Each snapshot in the fine tendency dataset was *coarse-grained*, reducing its spatial resolution to that of the coarse model. The nature of the coarse-graining algorithm warrants special attention and is discussed separately in § 4.2.

4. The same coarse-graining algorithm was applied to the first fine state snapshot in each pair from Step 1, producing a dataset of *coarse states*.

5. Each coarse state was input as an initial condition for the coarse model, the coarse model integrated for one time step only, and the resulting state saved. There were now [TODO:] pairs of coarse state snapshots separated by 3 time units, analogous to the fine state snapshots from Step 1.

6. Step 2 was repeated for the coarse state snapshots, producing a dataset of *coarse tendencies* (i.e., the time derivatives predicted by the coarse model).

7. Finally, the coarse tendencies were subtracted from the coarse-grained fine tendencies, producing the *subgrid tendencies*.

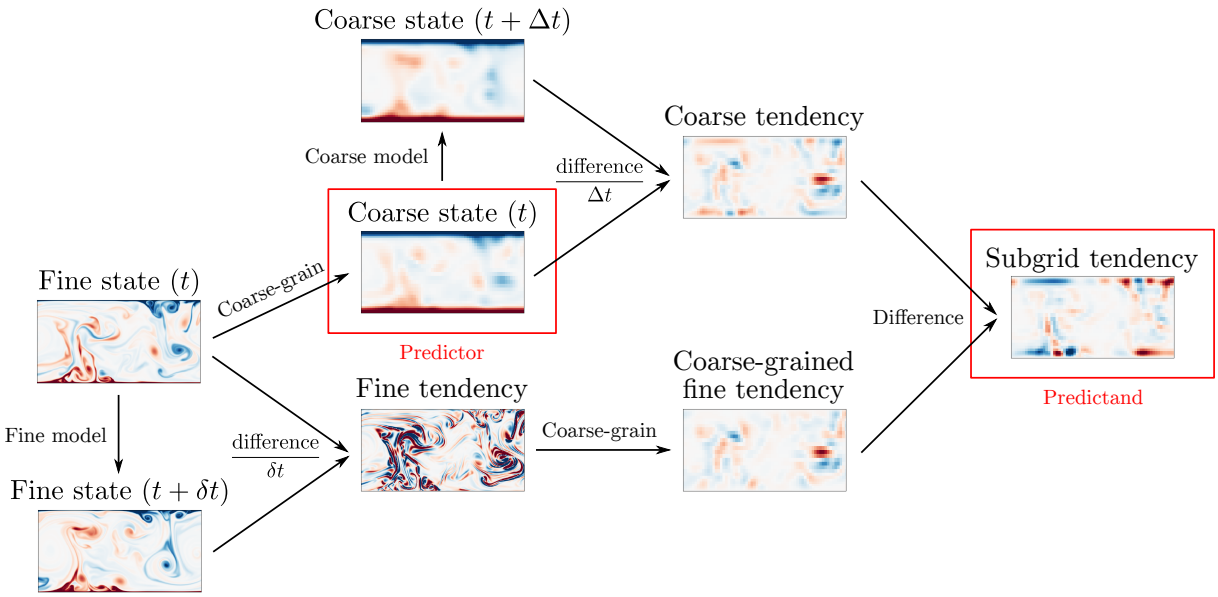

Figure 4.1: Flowchart illustrating the procedure used to calculate subgrid tendencies. The plots show an example of the workflow being applied to the temperature data and are for illustrative purposes only.

4.2 Choice of coarse-graining method

Coarse-graining is the process of reducing a gridded dataset onto a lower-resolution grid, and it is required at two points in the subgrid tendency calculation workflow: first to produce the coarse-grained fine tendency and then to produce the coarse state. It was found that the choice of coarse-graining method was a major influence on the quality of the calculated subgrid tendencies; this is the consequence of a subtle issue that initially seems purely philosophical but in fact has important practical consequences.

Broadly speaking, the output of a coarse (i.e., reduced-order) model is meant to approximate a certain *representation* of the output of the original fine model. To give three concrete examples, the coarse model might seek to reproduce (a) the values of the high-resolution fields on a sparser grid of points, or (b) the averages over a set of larger grid boxes, or (c) the first N Fourier coefficients (where N is less than the number of coefficients needed to fully determine the original field). The modeller has the freedom choose a representation, which in turn determines how the output of the coarse model should be interpreted. The choice of representation also implicitly determines a coarse-graining operation: a map from the state space of the fine model to the state space of the coarse model that isolates the necessary large-scale information and discards the rest. Referring to the previous examples, option (a) calls for an operation that simply discards, say, three out of every four or nine out of ten grid points. Option (b) calls for the grouping and averaging of the grid points that lie within each large grid box. Option (c) calls for the truncation of fine fields at the Nth coefficient in Fourier space.

The key lesson that was learnt during the course of this work is that the chosen representation and coarse-graining method must be appropriate to the nature of the coarse model. In this work, the coarse model was a Dedalus solver that, in Step 5 of the workflow in § 4.1, received gridded initial condition data in real space and integrated the governing equations forward in time using the same numerical method as the fine model. This gave rise to two constraints on the coarse-graining method:

1. The coarse-grained initial condition must be well-resolved on the coarse model's grid. Numerical solution algorithms for PDEs assume (e.g., by approximating derivatives as finite differences) that the solution is well-resolved on the discrete model grid, and can become unstable or produce output marred by artefacts if this condition is not met.

2. The initial condition must respect physical constraints, namely the divergence-free condition (3.9) and the boundary conditions (3.10)–(3.12). A numerical algorithm cannot be expected to behave predictably when presented with unphysical initial conditions.

During the development of this study, before the above requirements were known, coarse-graining was performed by averaging the fine grid points that lay within each coarse grid box (a method known within the Earth sciences as *first-order conservative regridding* because it preserves mean values). Figure `TODO: figure comparing coarse-graining methods`, illustrating the application of first-order conservative regridding to sample temperature data, demonstrates that the result is not very well-resolved on the coarse grid; in many places, adjacent grid points have sharp differences in temperature. First-order conservative regridding is also not guaranteed to preserve boundary values or the divergence-free nature of the velocity field. Consequently, the tendencies obtained from the coarse model in Step 6 of the workflow suffered from noise and numerical artefacts that propagated to the subgrid tendencies in Step 7. With the signal of interest obscured, it was impossible to model the subgrid tendencies as functions of the coarse state.

This issue was remedied using a new coarse-graining method. Consider the new set of PDEs

$$\frac{\partial \boldsymbol{u}}{\partial t} = -\boldsymbol{\nabla}\pi + \nabla^2 \boldsymbol{u}, \tag{4.1}$$

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta, \quad \text{and} \tag{4.2}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \tag{4.3}$$

subject to the required boundary conditions (3.10)–(3.12). (4.2) is simply a heat equation; over time, its initial condition is "smoothed", akin to the conduction of heat through the fluid in the absence of advection. (4.1) is the same except for the addition of the "pressure" term $-\boldsymbol{\nabla}\pi$, which provides an additional degree of freedom that is needed to simultaneously enforce the divergence-free condition. (4.3). The properties of these equations motivated the construction of a Dedalus model to solve them on the same grid as the fine model.

4.3 Analysis of subgrid tendencies

4.4 Modelling of subgrid tendencies