

DEPARTMENT OF MATHEMATICS

The Spectral Lagrange-Galerkin Method for
the Atmospheric Transportation of a Pollutant!

Part III. The Atmospheric Transportation of a Pollutant!

A. Priestley

Numerical Analysis Report 9/89

UNIVERSITY OF READING

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The work reported here forms part of the research programme of the Reading/Oxford Institute for Computational Fluid Dynamics and has been supported by the S.E.R.C. under grant number GR/E72256.

1. Introduction

Rather optimistically the first of these three reports referred to the "Atmospheric Transportation of Pollutants". In this, the final of these reports, we do actually get around to this goal.

The method described in the first report and shown to be highly promising (Priestley (1989)) is now applied to a three-dimensional problem - the transportation of a passive pollutant in the atmosphere.

In the following section the test problem is described and the results presented. In Section 3 we will discuss how to improve on these results and where future work might best be expended.

In the Appendix we include a discussion on monotone cubic interpolation because this is an important point if a spectral representation is not used in the vertical. Williamson & Rasch (1989) and Rasch & Williamson (1989) have studied a much wider class of polynomial interpolation. However, the analysis presented here is a little different, and an alternative estimate to the derivatives is presented.

Acknowledgements

Many thanks must go to Dr. Mike Blackburn and Kevin Dunn of the Meteorology Department at the University of Reading for their help with this work and particularly in supplying the velocity fields for the transportation problem.

2. The Test Problem

For the test problem we study the advection of a pollutant in the Earth's atmosphere over a period of 5 days. The pollutant is assumed to be passive, that is, it is transported by the winds but it does not affect the weather itself. The initial pollutant distribution is taken to be the value of the humidity at the start of the 5 day period. The winds were calculated using a standard numerical weather prediction model. Since the problem concerns only a passive pollutant these winds can be stored and used as data for the velocity field governing the transportation of the pollutant by the spectral Lagrange-Galerkin method.

In the horizontal a T21 spectral model is used and 19 levels are used in the vertical, level 19 being closest to the Earth's surface.

The time-steps were $\frac{1}{4}$ of an hour in the numerical weather prediction code but the velocity fields were only output every other time-step as the spectral Lagrange-Galerkin method used time-steps of $\frac{1}{2}$ hours. The reason for this was due to a lack of storage but it does at least serve to demonstrate that much longer time-steps can be used with Lagrangian schemes than with the more conventional methods

Figures 1a-1e are contour plots of humidity at day 0. The contours are plotted at intervals of 2 grams/kg water/air. Figures 2a-2e show the solution at day 5 as predicted by a conventional spectral method in the horizontal and a second order centred finite difference approximation in the vertical using $\frac{1}{4}$ hour time-steps.

One of the first things to notice about these results is the fact that maximum values of humidity have been well maintained. However, having said this we see that the minimum value has not been preserved at all. The minimum value of humidity should, of course, be zero but is in

fact slightly negative due to noise in the initial data. The solution produced by the standard spectral approach with a finite difference approximation in the vertical has resulted in considerable undershoot, particularly in levels 17 & 19 - figures 2d & 2e. Noise also seems to be a significant problem on levels 13 & 15, see figures 2b & 2c.

The results for the spectral Lagrange-Galerkin, with twice the time-step of the above results, are shown in Figures 3a-3e. There are good points and bad points connected with these pictures. Firstly we note that the results, particularly at the lowest level, compare well with Figure 2 in that the positions of the maximum coincide and that there is a degree of similarity between the position and shape of the major features - especially if we take into account the amount of noise present in the results depicted in Figure 2.

Although the position of the maximum is predicted to be in the same position by both codes the value of the maximum is quite different. This is the fault of the spectral Lagrange-Galerkin method and is caused by the sharp gradient in the concentration of the pollutant - around the Himalayas as it happens. This phenomenon, which is worse than a purely Gibbs' phenomenon would cause does improve as more modes are used to represent the solution.

There is no undershoot, at any level, indeed the solution does seem to have been smoothed out somewhat to give the minima that appear in Figure 3. This is almost entirely due to the vertical approximation used. Between levels a simple linear interpolation was used which is a first-order, extremely diffusive, scheme. This was used essentially because it was so simple but will obviously need to be replaced in the future.

3. Conclusions

We have shown that the spectral Lagrange-Galerkin method is a very promising method for transportation problems in the atmosphere.

The most obvious thing that needs to be changed is the way the vertical co-ordinate is dealt with. Either a spectral representation is required in the vertical or we could perhaps change to the direct spectral Lagrange-Galerkin method, where we look backwards along the trajectory, and use a data-dependent monotone cubic interpolation. Indeed, it may even be possible to do something similar with the weak method where we look forward in time along the trajectory.

At the moment the trajectories have just been approximated by straight lines in (λ, μ, η) space. This does not seem to have caused any undue problems but we could probably benefit from the ideas of Williamson & Rasch (1989) and Côté (1988).

A spectral Lagrangian method is always going to be more expensive than a finite difference Lagrangian method. Naturally we hope to obtain spectral accuracy but it would be welcome if the expense could be reduced. There are two spectral transformations that we need to do at each time-step. With the weak method we firstly perform an inverse transformation to obtain gridpoint values of the function. At the other end of the trajectory we then project back into spectral space. The first part can be formed very quickly because we can use a fast Fourier transform and, since the grid is fixed, much information can be calculated once and for all and then stored. This is not the case at the other end of the trajectory where we will usually fall between gridpoints and have to calculate the spectral decomposition at each point at each time-step.

A way around this would be to use the non-interpolatory approach, see Ritchie (1986).

In using this procedure we ensure that our trajectory always ends at a gridpoint. This would then mean we could transform into spectral space very quickly using the fast Fourier transform and stored information.

Level number 11

Maximum = 4.69

Minimum = -0.30

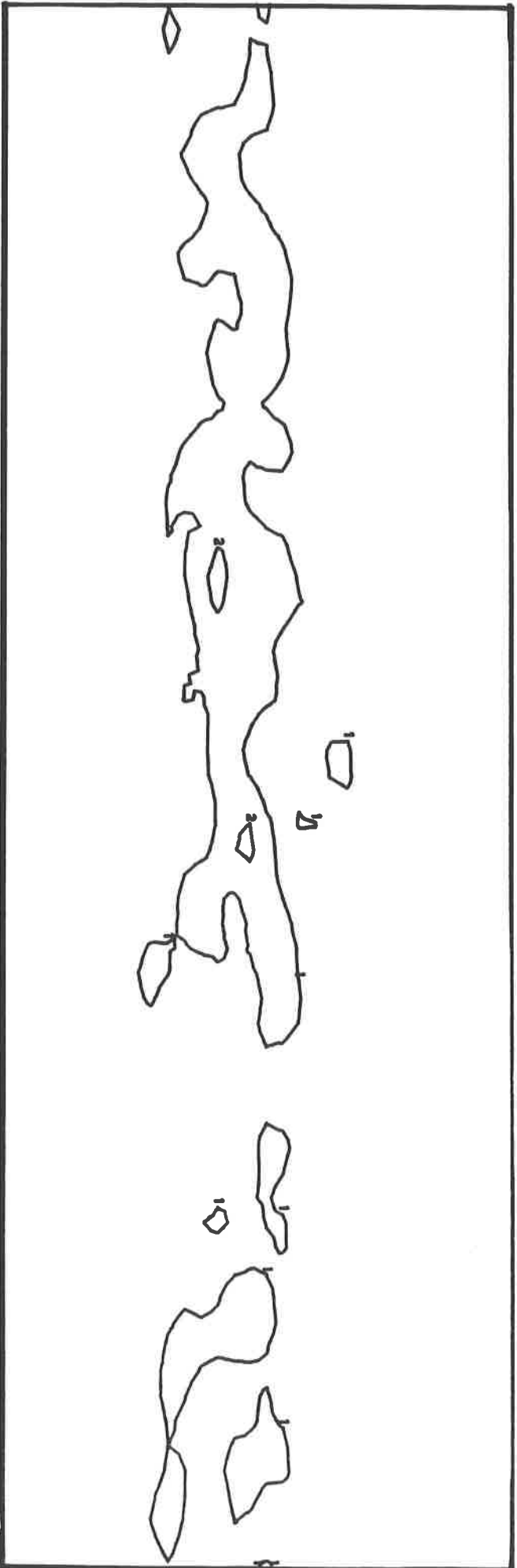


Figure 1a Pollutant Day 0

Level number 13

Maximum = 8.00

Minimum = -0.36

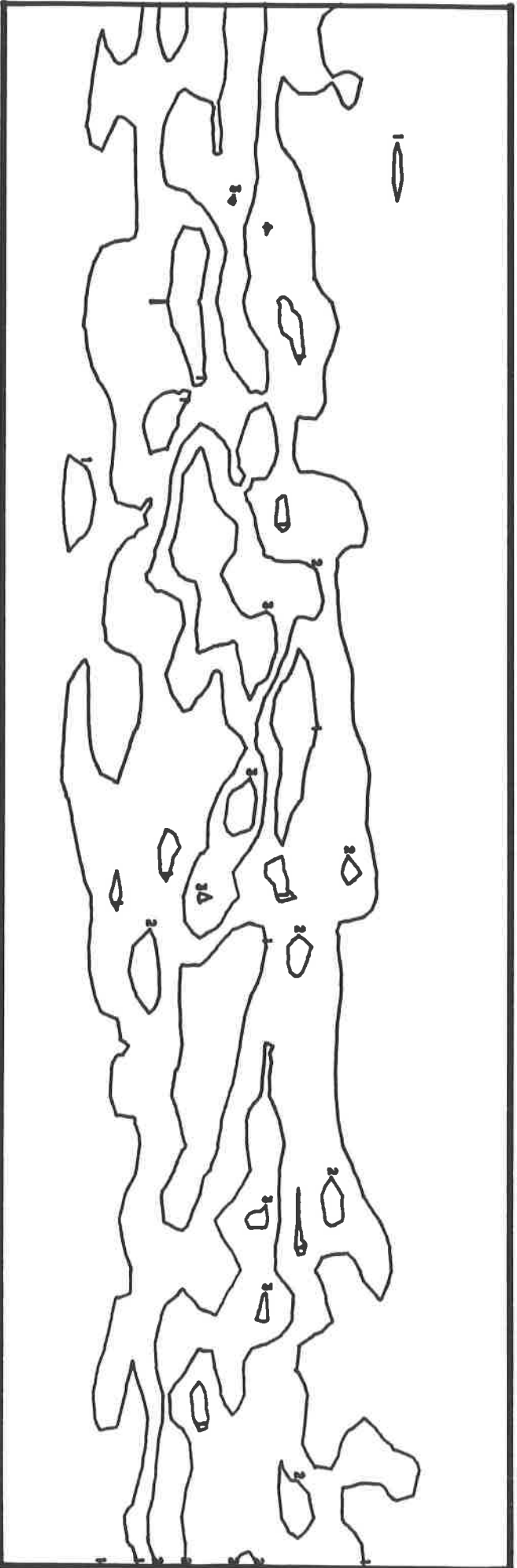


Figure 1b Pollutant Day 0

Level number 15

Maximum = 15.27

Minimum = -0.37

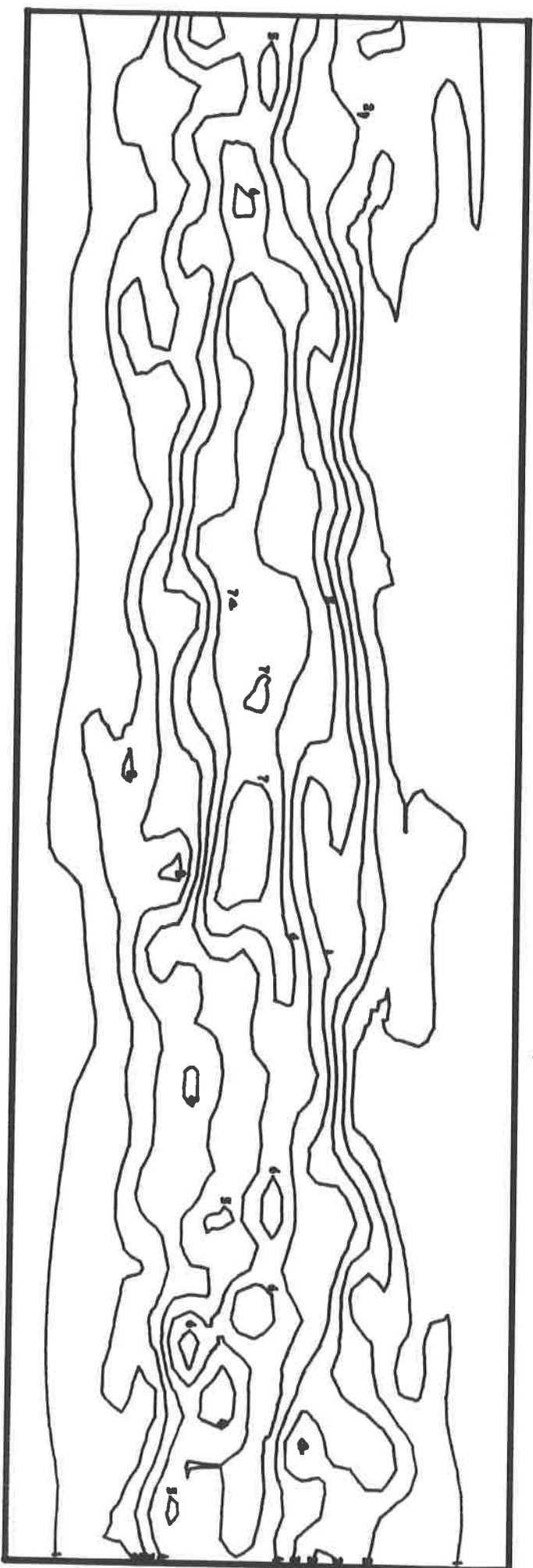


Figure 1c Pollutant Day 0

Level number 17

Maximum = 19.58

Minimum = -0.61

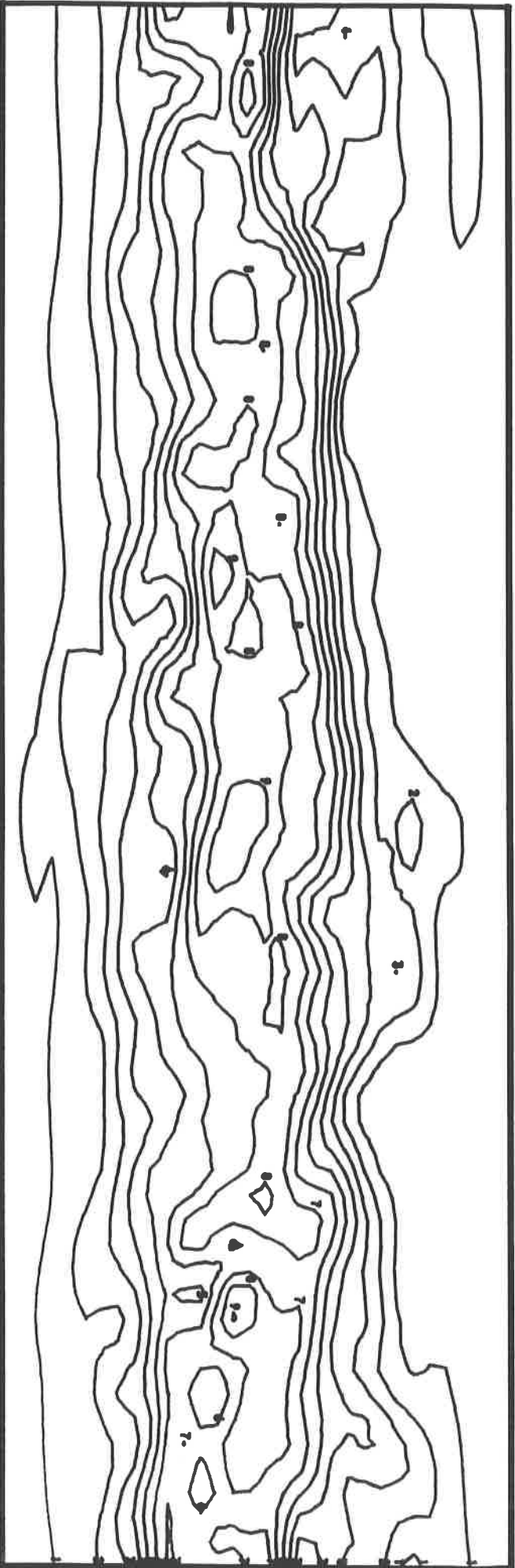


Figure 1d Pollutant Day 0

Level number 19

Maximum = 21.77

Minimum = -0.55

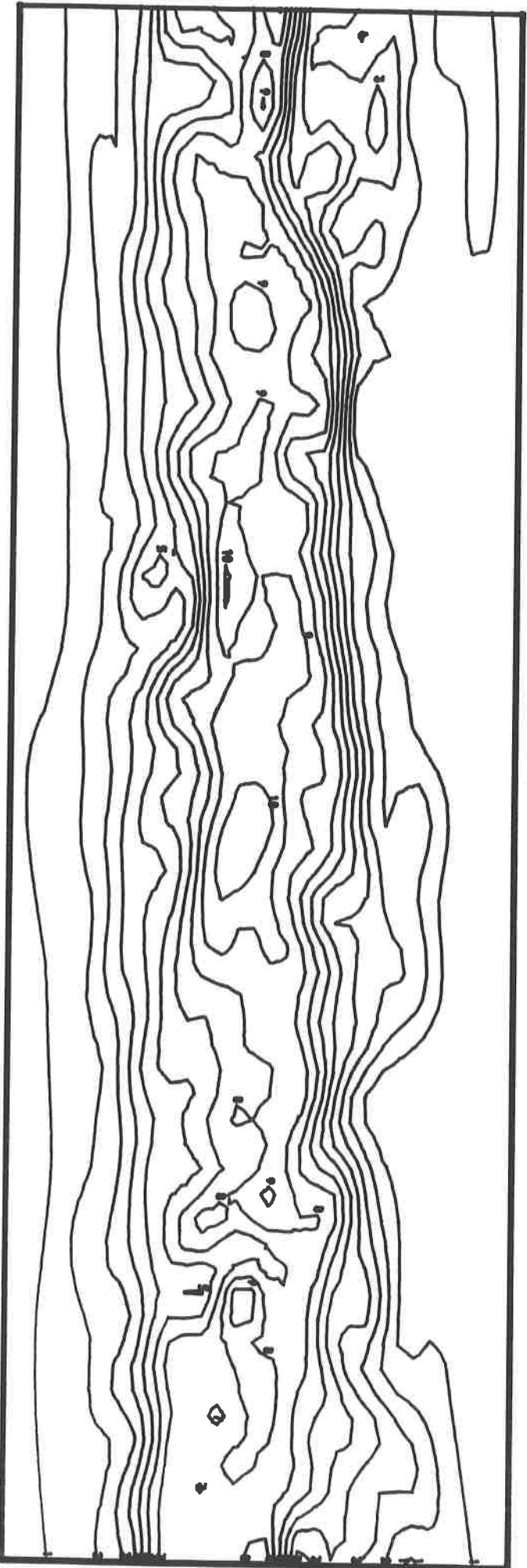


Figure 1e Pollutant Day 0

Level number 11

Maximum = 5.65

Minimum = -0.47

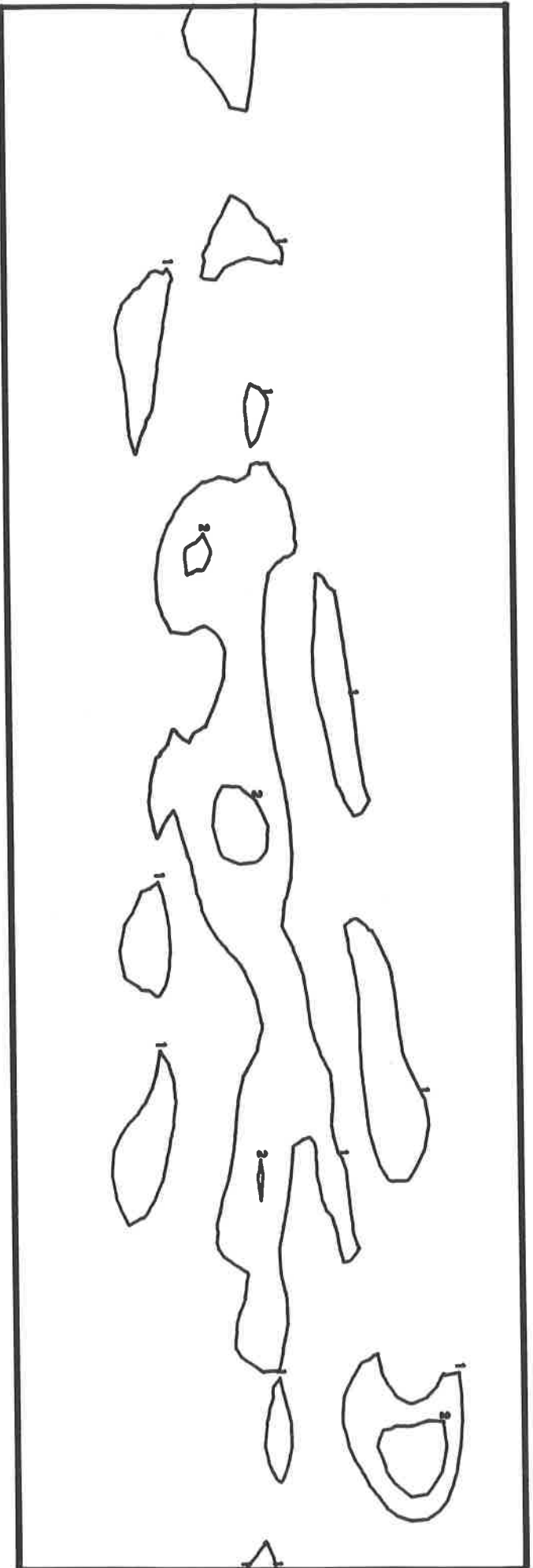


Figure 2a Day 5

Level number 13

Maximum = 9.11

Minimum = -0.85

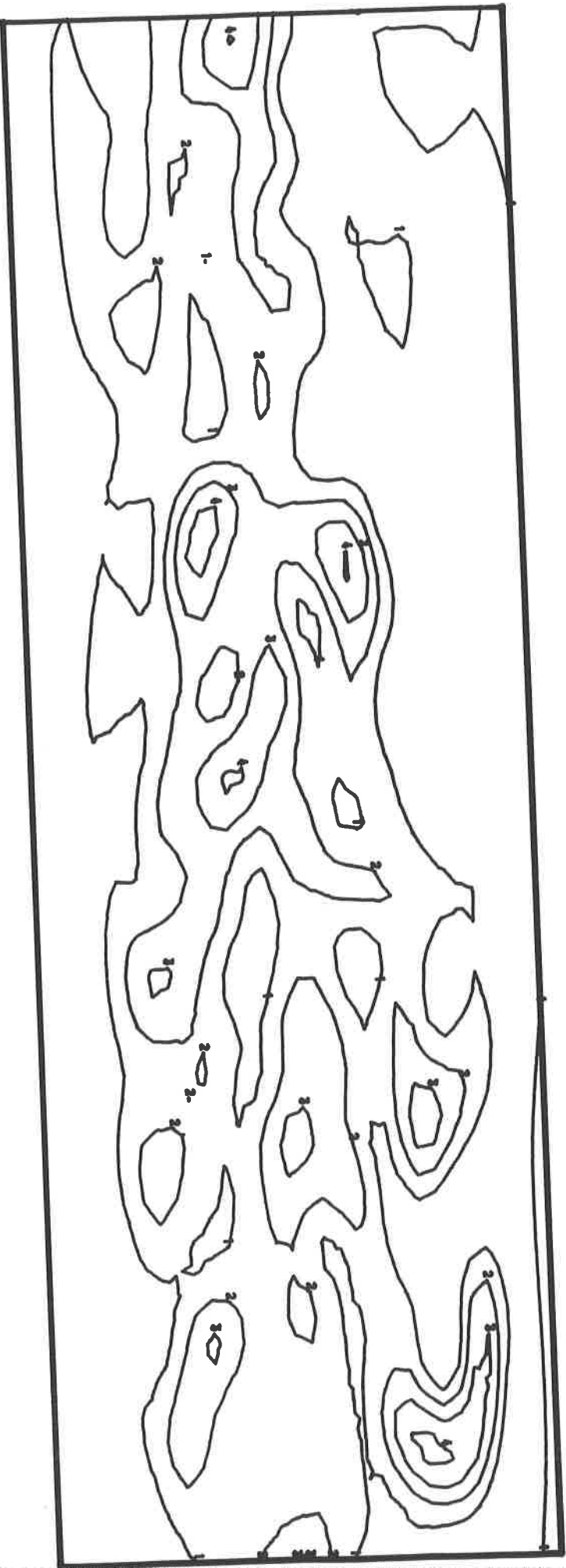


Figure 2b Day 5

Level number 15

Maximum = 16.93

Minimum = -2.20

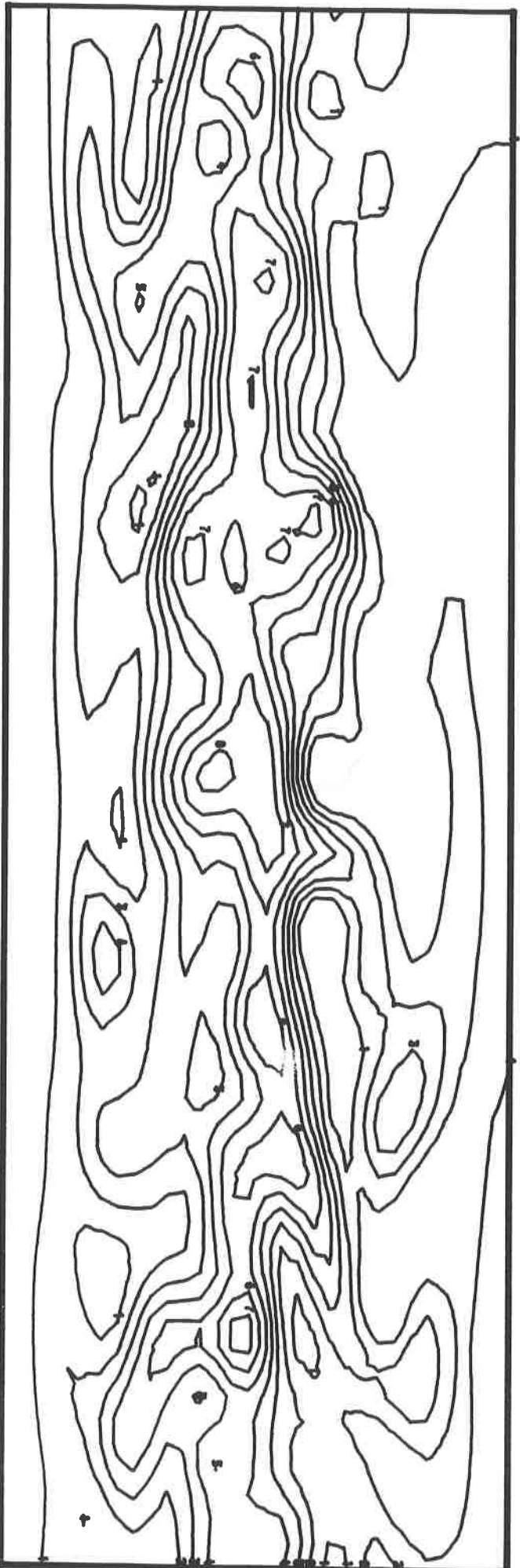


Figure 2c Day 5

Level number 17

Maximum = 20.26

Minimum = -4.14

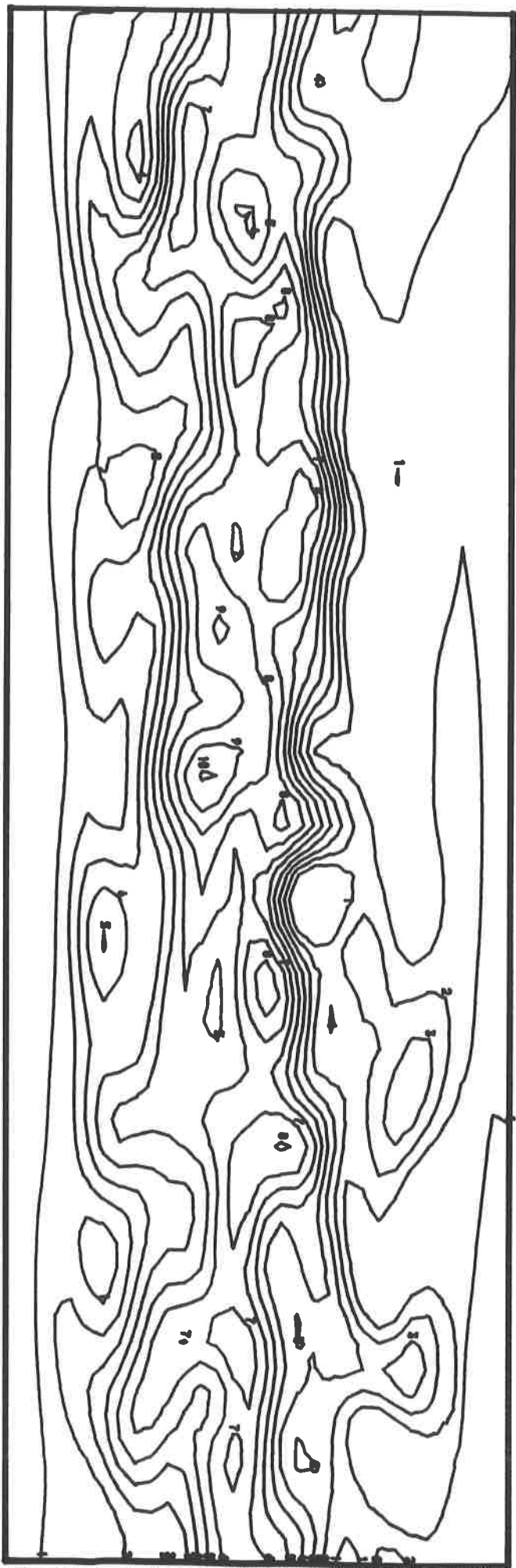


Figure 2d Day 5

Level number 19

Maximum = 20.37

Minimum = -3.40

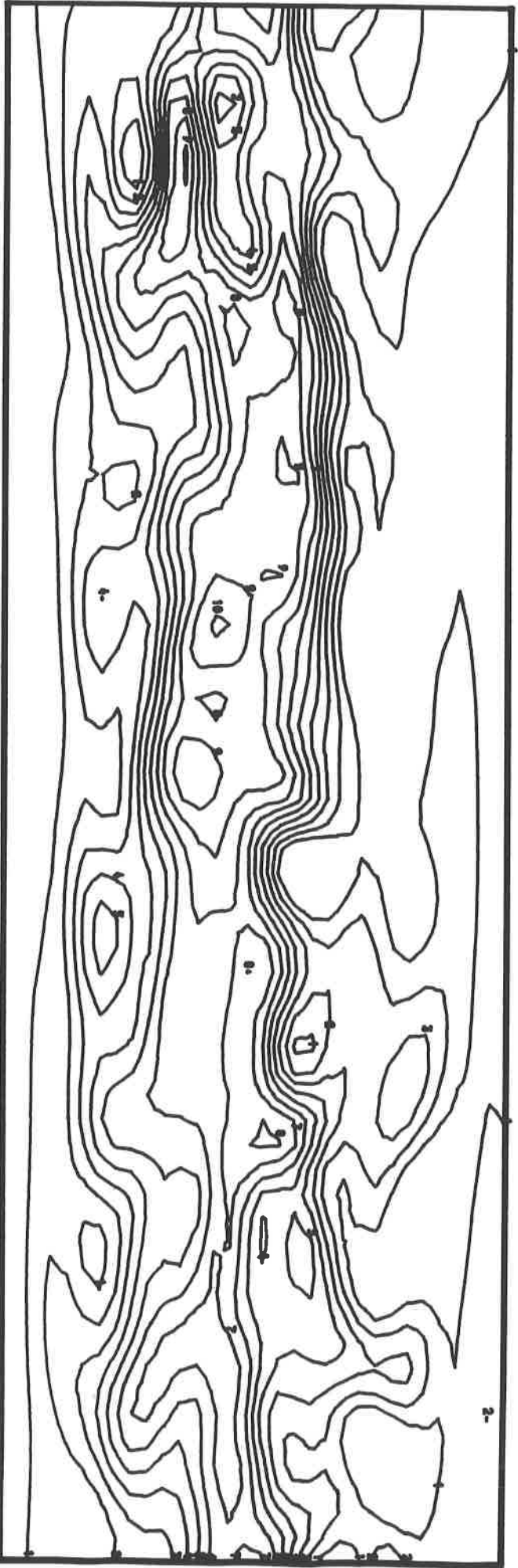


Figure 2e Day 5

Level number 11

Maximum = 2.90

Minimum = 0.30

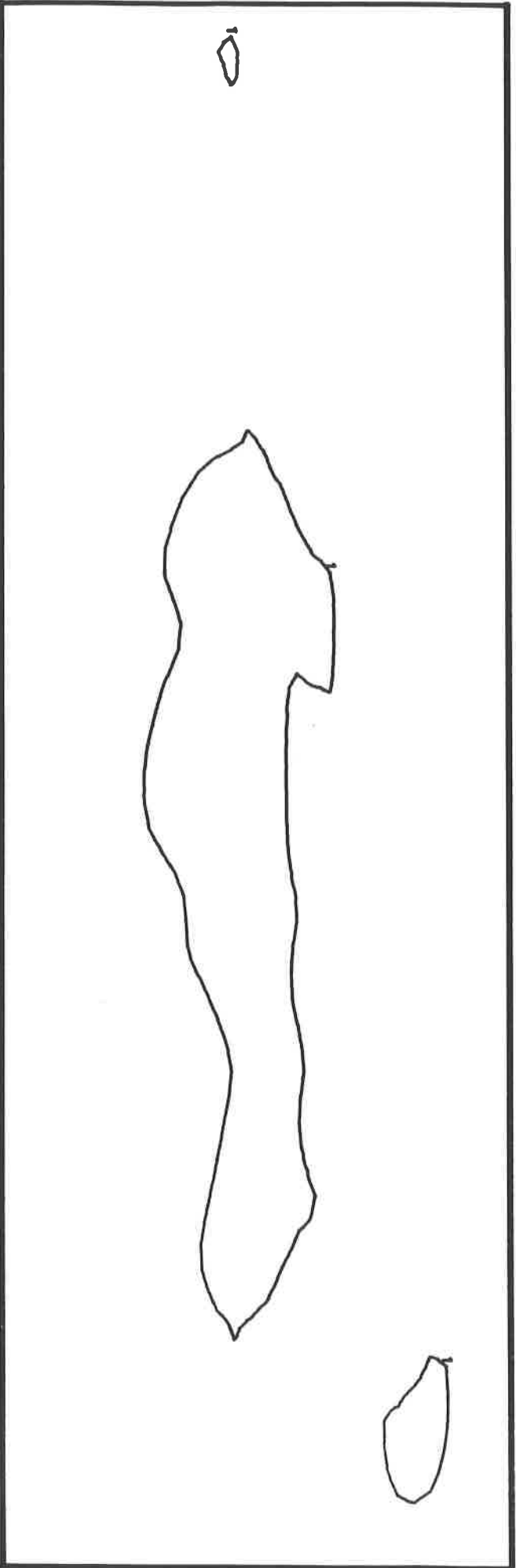


Figure 3a Day 5 Spectral Lagrange-Galerkin

Level number 13

Maximum = 6.41

Minimum = 0.58

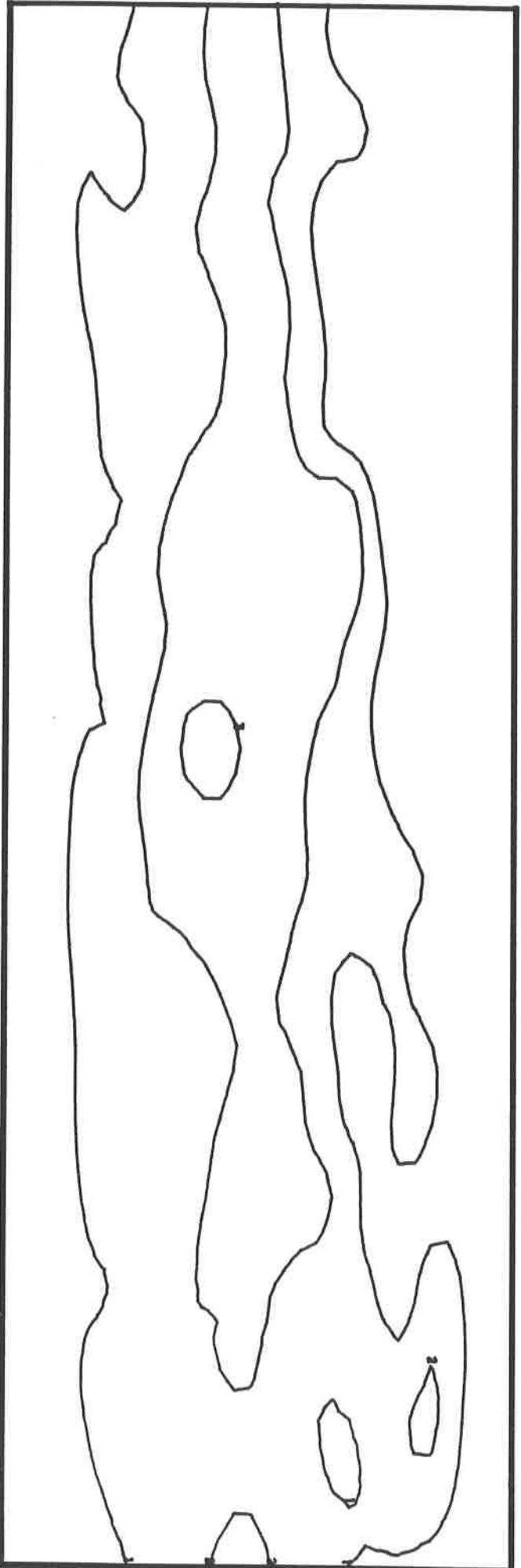


Figure 3b Day 5 Spectral Lagrange-Galerkin

Level number 15

Maximum = 12.27

Minimum = 0.63

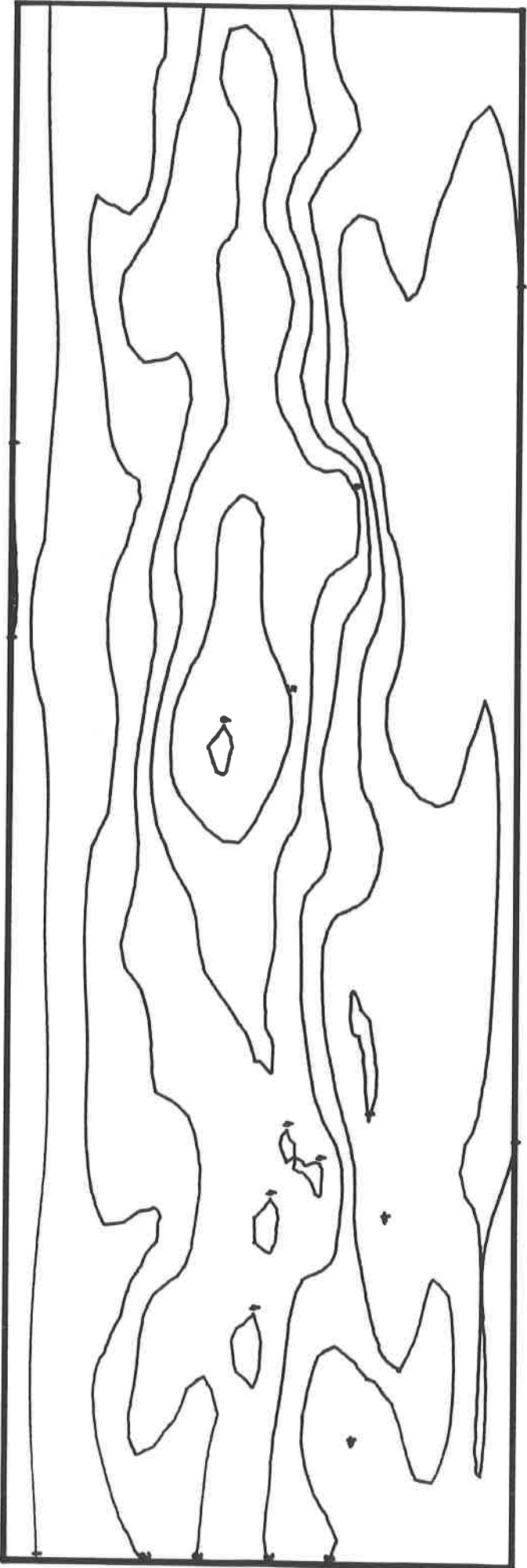


Figure 3c Day 5 Spectral Lagrange-Galerkin

Level number 17

Maximum = 17.12

Minimum = 0.49

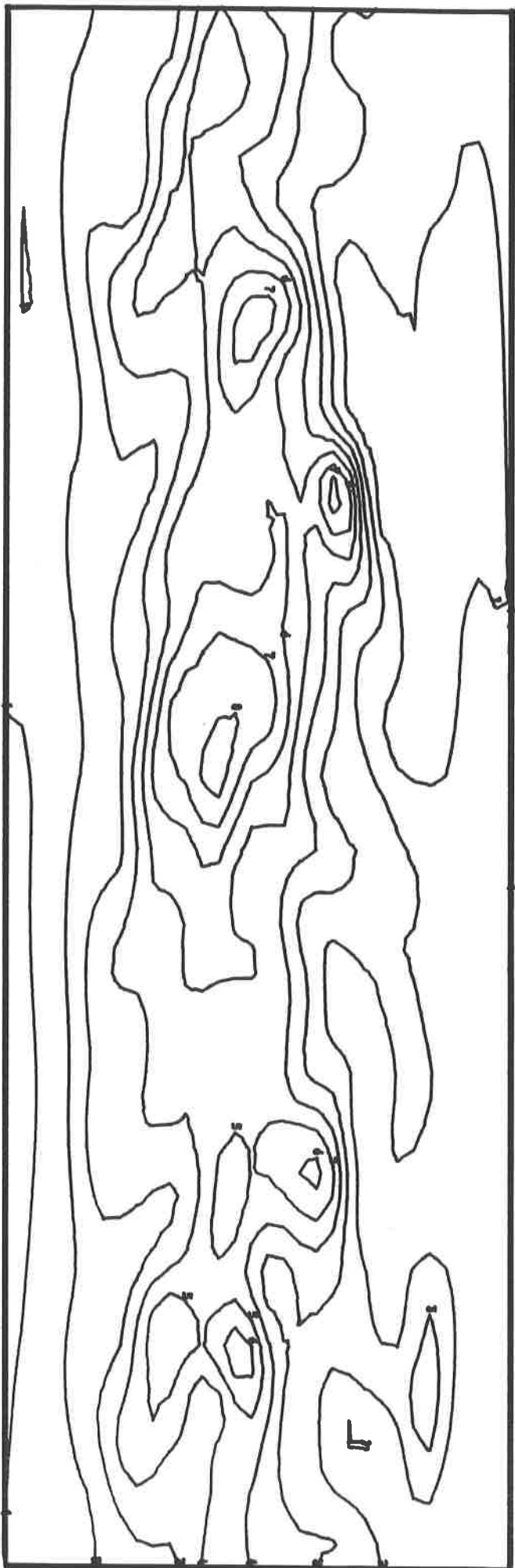


Figure 3d Day 5 Spectral Lagrange-Galerkin

Level number 19

Maximum = 25.82

Minimum = 2.03

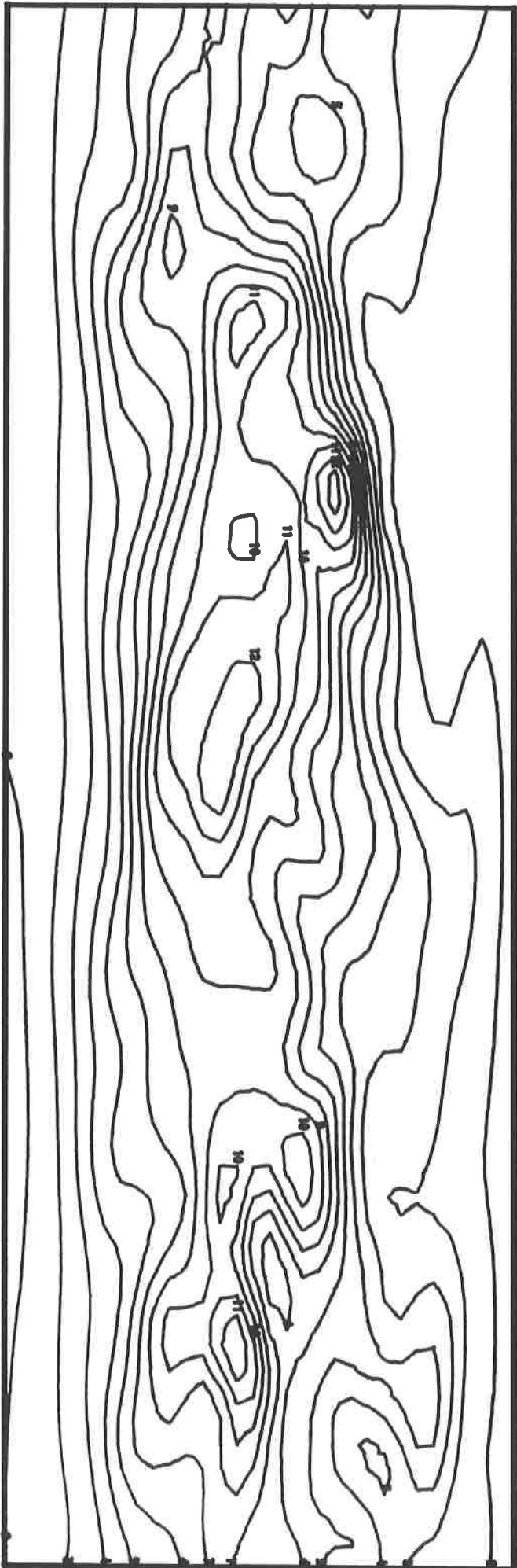


Figure 3e Day 5 Spectral Lagrange-Galerkin

Appendix

The Search for SPOC - The Supreme Piecewise Oscillation-free Cubic.

As we have mentioned earlier the linear interpolation used in the vertical introduces an unacceptable amount of diffusion. One way around this problem is to use a higher order polynomial interpolant. One good point about the linear interpolant is the fact that it is monotone and this is a constraint we shall want to keep with the cubics.

Using the notation of Fritsch and Carlson (1980) we consider a cubic polynomial function $p(x)$ on the interval $[x_i, x_{i+1}]$ such that $p(x)$ is monotone and

$$\begin{aligned} p(x_i) &= f_i \\ p(x_{i+1}) &= f_{i+1} . \end{aligned}$$

We can write $p(x)$ on each sub-interval in terms of the cubic Hermite basis functions to obtain

$$p(x) = f_i H_1(x) + f_{i+1} H_2(x) + d_i H_3(x) + d_{i+1} H_4(x)$$

where

$$\begin{aligned} d_j &= p'(x_j) \quad j = i, i+1 \\ H_1(x) &= \phi((x_{i+1} - x) / h_i) , \\ H_2(x) &= \phi((x - x_i) / h_i) , \\ H_3(x) &= -h_i \psi((x_{i+1} - x) / h_i) , \\ H_4(x) &= h_i \psi((x - x_i) / h_i) , \end{aligned}$$

with

$$\begin{aligned} h_i &= x_{i+1} - x_i , \\ \phi(t) &= 3t^2 - 2t^3 , \\ \text{and } \psi(t) &= t^3 - t^2 . \end{aligned}$$

Letting $\Delta_i = (F_{i+1} - F_i) / h_i$ we can rewrite the Hermite cubic polynomial as

$$\begin{aligned} p(x) &= \left[\frac{d_i + d_{i+1} - 2\Delta_i}{h_i^2} \right] (x - x_i)^3 + \left[\frac{-2d_i - d_{i+1} + 3\Delta_i}{h_i} \right] (x - x_i)^2 \\ &+ d_i(x - x_i) + f_i . \end{aligned} \tag{A1}$$

As it stands (A1) will not be monotonic. Monotonicity is ensured by limiting the values of d_i and d_{i+1} . An obvious necessary condition for monotonicity is that

$$\text{sign}(d_i) = \text{sign}(d_{i+1}) = \text{sign}(\Delta_i) . \tag{A2}$$

Writing $\alpha = d_i/\Delta_i$ and $\beta = d_{i+1}/\Delta_i$, $\Delta_i \neq 0$, Fritsch and Carlson (1980) were able to prove that (A1) is always monotone if and only if (A2) holds in conjunction with one or both of the following conditions on (α, β) : -

$$0 \leq \alpha \leq 3 , \quad 0 \leq \beta \leq 3 \tag{A3a}$$

$$\text{and} \quad \phi(\alpha, \beta) \leq 0 \tag{A3b}$$

where

$$\phi(\alpha, \beta) = (\alpha-1)^2 + (\alpha-1)(\beta-1) + (\beta-1)^2 - 3(\alpha+\beta-2) .$$

For obvious reasons (A3a) is the more usually applied constraint.

This still leaves us with the question of how to choose the estimates of the derivatives. As mentioned in the introduction Williamson & Rasch (1989) and Rasch & Williamson (1989) have performed exhaustive tests on the choices of derivatives and on the type of polynomial. Here we will only consider cubic polynomials but will provide some analytic results for the various choices of derivative estimate.

The derivative estimates chosen were: -

$$\text{Linear} \quad d_i = \begin{cases} \Delta_i & x \in (x_i, x_{i+1}) \\ \Delta_{i-1} & x \in (x_{i-1}, x_i) \end{cases}$$

$$\text{Central Difference or Arithmetic Mean} \quad d_i = \frac{(\Delta_{i-1} + \Delta_i)}{2}$$

$$\text{Cubic} \quad d_i = \begin{cases} \frac{(2\Delta_{i-1} + 5\Delta_i - \Delta_{i+1})}{6} & x \in (x_i, x_{i+1}) \\ \frac{(-\Delta_{i-2} + 5\Delta_{i-1} + 2\Delta_i)}{6} & x \in (x_{i-1}, x_i) \end{cases}$$

$$\text{Hyman} \quad d_i = \frac{-\Delta_{i-2} + 7\Delta_{i-1} + 7\Delta_i - \Delta_{i+1}}{12}$$

and

$$\text{MAHG} \quad d_i = \frac{-3\Delta_{i-2} + 19\Delta_{i-1} + 19\Delta_i - 3\Delta_{i+1}}{32}$$

The two quantities that we will study are phase speed and amplification factor for the linear advection equation

$$u_t + au_x = 0 \quad (\text{A4})$$

The phase speed should equal a and the amplification factor should be unity. The errors in these quantities are averaged over all CFL numbers and all wave numbers. These results are then compared to those obtained for the linear derivative estimate, except for schemes with higher order phase accuracy which are then compared to the phase accuracy of the cubic derivative.

We start by doing the analysis in some detail for the linear derivative estimate.

In calculating the phase speed of equation (A4) we look for solutions of the form

$$u(x, t) = e^{i(\omega t - \xi x)} \quad (\text{A5})$$

where for every real wave number ξ we assume that there is a corresponding real value of the frequency ω such that (A5) is a solution to (A4). The relation $\omega = \omega(\xi)$ is called the dispersion relation for the differential equation. The phase speed is then defined as

$$c(\xi) = \omega(\xi)/\xi .$$

When using a numerical scheme, (A5) is replaced by

$$U_i^n = e^{i(\omega n \Delta t - \xi_j \Delta x)} . \quad (\text{A6})$$

Linear

For the linear derivative estimate

$$c_{\text{linear}}(\xi) = \frac{\arcsin \left[\frac{\sin(\Delta x \xi) a \Delta t}{\Delta x} \right]}{\Delta t \xi} . \quad (\text{A7})$$

Equation (A7) is a little unwieldy to deal with so the phase speed is expanded as a Taylor series in ξ to produce

$$c_{\text{linear}}(\xi) \approx a - \frac{a}{6} (-a^2 \Delta t^2 + \Delta x^2) \xi^2 + \frac{a}{120} (-10a^2 \Delta t^2 \Delta x^2 + 9a^4 \Delta t^4 + \Delta x^4) \xi^4 .$$

(A8)

In comparing with the other schemes we shall look at the ratios of their respective ξ^2 terms squared and then integrate over all CFL numbers between 0 and 1. For the schemes with a higher order phase accuracy we compare the ξ^4 terms to those of the cubic derivative estimate.

The amplification factor for this scheme is

$$|\lambda|_{\text{linear}}^2 = 1 - 4s^2\nu + 4\nu^2s^2 ,$$

where ν is the CFL number and $s^2 = \sin^2(\xi/2)$. The measure of the error here is calculated as

$$\int_0^1 \int_0^1 (1 - |\lambda|^2)^2 d\nu ds^2 .$$

By definition both the phase speed error and the amplification error are 100%.

Central Differencing

$$c_{cd}(\xi) = \frac{\arcsin \left[\frac{\sin(\Delta x \xi) a \Delta t (\Delta x a \Delta t + \Delta x^2 - a^2 \Delta t^2) + \cos(\Delta x \xi) a^2 \Delta t^2 - \cos(\Delta x \xi) \Delta x a \Delta t}{\Delta x^3} \right]}{\Delta t \xi}$$

$$c_{cd}(\xi) \approx a - \frac{a}{6} (2a^2 \Delta t^2 - 3\Delta x a \Delta t + \Delta x^2) \xi^2 + \frac{a}{120} (30a^3 \Delta t^3 \Delta x - 21a^4 \Delta t^4 + 5a^2 \Delta x^2 \Delta t^2 - 15a \Delta x^3 \Delta t + \Delta x^4) \xi^4 .$$

The comparative phase speed error is 18.22% that of the linear estimate.

$$|\lambda|_{cd}^2 = (-16v^3 - 48v^5 + 48v^4 + 16v^6)s^6 + (-12v^2 + 24v^3 - 12v^4)s^4 + 1.$$

The amplification error is 40.41% that of the linear scheme.

Cubic

$$c_{cubic}(\xi) = \frac{-\arcsin \left[\frac{\sin(\Delta x \xi) a \Delta t (a^2 \Delta t^2 - 4\Delta x^2 - \cos(\Delta x \xi) a^2 \Delta t^2 + \cos(\Delta x \xi) a^2 \Delta t^2)}{3\Delta x^3} \right]}{\Delta t \xi}$$

$$c_{cubic}(\xi) \approx a - \frac{a}{120} (a^4 \Delta t^4 + 4\Delta x^4 - 5\Delta x^2 a^2 \Delta t^2) \xi^4 + \frac{a}{1008} (-21\Delta x^4 a^2 \Delta t^2 + 21a^4 \Delta t^4 \Delta x^2 - 4a^6 \Delta t^6 + 4\Delta x^6) \xi^6 .$$

This has third-order accurate phase speed and again, by definition, we say that its comparative phase error is 100%.

$$|\lambda|_{\text{cubic}}^2 = 1 + \frac{4}{9} s^4 v (v+1)(v-1)(v-2)(4s^2 v^2 - 4s^2 v - 3)$$

resulting in an amplification error of 50.38% of that of the linear scheme.

Hyman

$$c_{\text{Hyman}}(\xi) = \frac{1}{\Delta t \xi} \arcsin \left[\frac{1}{3\Delta x^3} \sin(\Delta x \xi) a \Delta t \left(-2 \cos(\xi \Delta x) a \Delta x \Delta t \right. \right. \\ \left. \left. - \cos(\xi \Delta x)^2 a^2 \Delta t^2 + a \Delta x \Delta t + \cos(\xi \Delta x)^2 a \Delta x \Delta t + 4\Delta x^2 \right. \right. \\ \left. \left. - \cos(\xi \Delta x) \Delta x^2 + 3 \cos(3\Delta x)^2 a^2 \Delta t^2 - 2a^2 \Delta t^2 \right) \right]$$

$$c_{\text{Hyman}}(\xi) \approx a - \frac{a}{120} (a^4 \Delta t^4 + 5\Delta x^2 a^2 \Delta t^2 - 10\Delta x^3 a \Delta t \\ + 4\Delta x^4) \xi^4 \\ + \frac{a}{1008} (-21a^4 \Delta t^4 \Delta x^2 + 4\Delta x^3 a^3 \Delta t^3 + 7\Delta x^4 a^2 \Delta t^2 - 4a^6 \Delta t^6 \\ - 28\Delta x^5 a \Delta t + 4\Delta x^6) \xi^6$$

Comparing with the cubic scheme this has 22.07% of the phase error.

$$|\lambda|_{\text{Hyman}}^2 = 1 + \frac{4}{9} s^4 v^2 (v-1)^2 (16s^6 v^2 - 16vs^6 + 16s^4 v^2 - 16vs^4 - 4s^4 + 4s^2 v^2 - 4vs^2 - 20s^2 - 3) .$$

The amplification error is 19.03% that of the linear scheme.

MAHG

$$c_{\text{MAHG}}(\xi) = \frac{1}{\Delta t \xi} \arcsin \left[\frac{\sin(\xi \Delta x) a \Delta t}{8 \Delta x^3} (-5 \cos(\xi \Delta x) a \Delta x \Delta t + 2a \Delta x \Delta t + 3 \cos(\xi \Delta x)^2 a \Delta x \Delta t + 8 \cos(\xi \Delta x) a^2 \Delta t^2 - 3 \cos(\xi \Delta x)^2 a^2 \Delta t^2 - 3 \cos(\xi \Delta x) \Delta x^2 + 11 \Delta x^2 - 5a^2 \Delta t^2) \right]$$

$$c_{\text{MAHG}}(\xi) \approx a + \frac{a}{48} (2a^2 \Delta t^2 - 3a \Delta x \Delta t + \Delta x^2) \xi^2 - \frac{a}{960} (30a^3 \Delta t^3 \Delta x - 12a^4 \Delta t^4 + 50a^2 \Delta t^2 \Delta x^2 - 105a \Delta t \Delta x^3 + 37 \Delta x^4) \xi^4 .$$

This has a phase error of 0.28% compared to that of the linear scheme.

$$|\lambda|_{\text{MAHG}}^2 = 1 + \frac{1}{4} s^6 v^2 (1-v)^2 (36s^4 v^2 - 36s^4 v + 24s^2 v^2 - 24s^2 v - 9s^2 + 4v^2 - 4v - 39) .$$

This results in an amplification error of 27.77% that of the linear scheme.

| Scheme | Order Accuracy of Phase Speed | Phase error compared to linear | Phase error compared to cubic | Amplification error |
|--------------------|-------------------------------|--------------------------------|-------------------------------|---------------------|
| Linear | 1st | 100% | - | 100% |
| Central Difference | 1st | 18.22% | - | 40.41% |
| Cubic | 3rd | - | 100% | 50.38% |
| Hyman | 3rd | - | 22.07% | 29.03% |
| MAHG | 1st | 0.28% | - | 27.77% |

Table 1

Table 1 is useful for seeing that we would expect the central difference estimate to provide a better scheme than the linear derivative estimate, or that we would expect the Hyman derivative to provide us with a better scheme than the cubic derivative estimate. The problem is how do we compare the MAHG derivative estimate (which we believe to be original and which has the lowest amplification error) and the Hyman derivative estimate which has a formally more accurate phase speed. If we consider a derivative estimate at the point i that just involves the five points $i-2, i-1, i, i+1, i+2$ then the Hyman estimate gives the minimum amplification error for a scheme with 3rd order phase accuracy. If the 3rd order phase accuracy is relaxed then we can reduce the amplification error while still keeping a stable scheme, to obtain the MAHG derivative estimate.

Since Table 1 cannot tell us which scheme is best of these two, they were both applied to the linear advection of a square wave. The

derivatives were limited by (A3a). It must be stressed that these tests were not extensive but in the examples we did the MAHG derivative estimate always performed better although never reducing the error by more than 10%. It would be interesting to see how the MAHG derivative compared to the Hyman derivative in the much more challenging tests of Rasch & Williamson (1989).

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