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STOCHASTIC PREDICTION OF DETERMINISTIC MODELS

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1. INTRODUCTION

One can identify at least three basic reasons why we might choose to use stochastic models for describing geophysical phenomena. First, systems of interest may be subject to external forcing that we cannot define except in probabilistic terms. Then the behavior of the system, insofar as we are able to describe it, must be thought of as stochastic.

Second, the system may have a large number of interacting components that we cannot describe individually and in detail, so instead we view the statistical conglomeration of all the components and their interactions as a stochastic model. If there are enough components we may be able to formulate, in one sense, a deterministic description of the bulk behavior of the system, even though the model by which we generate that description is stochastic.

A third reason for choosing a stochastic model for a system is that the initial state of the system is frequently poorly known. In such a case there is an ensemble of possible initial states whose time-dependent behavior one might choose to follow. Instead of following any one ensemble member it is preferable to look at the entire ensemble in a collective, or, better, a stochastic framework. This enables one to say what he knows about future states of the system fully recognizing his uncertainties at the start.

These three reasons for constructing stochastic models are not in any sense exclusive. For example a model used for meteorological prediction might include diabatic effects, or boundary influences, that are treated by the first kind

of stochastic model, and the effects of convective processes or dissipation that may fall under the framework of the second class of stochastic process. Further our predictions depend on widely scattered imperfect observations making it subject to the third kind of stochastic treatment.

I have been particularly interested in this third aspect of stochastic modeling, so I will discuss its application to an otherwise deterministic system. Other speakers, I know, will describe other kinds of systems. I emphasize the difference that in the first two cases the geophysical system is itself stochastic and to some extent indeterminate. In the case with which I deal the only indeterminacy is in the mind of the investigator who is unable to define the initial state. In every real geophysical problem of a time-dependent nature, there will be some indeterminacy in the initial conditions. When it comes to making predictions this initial uncertainty must be borne in mind. Again the methods I use are applicable to systems that are themselves inherently stochastic, but in our example we apply them to a completely deterministic system for the sake of simplicity.

2. THE DETERMINISTIC MODEL

The particular system we use here to demonstrate and to test stochastic dynamic prediction consists of one-dimensional non-linear shallow water waves, chosen largely because we will all recognize the equations. Let us consider that our geophysical system is suitably represented by the partial differential equations

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} - g \frac{\partial h}{\partial x}$$

$$\frac{\partial h}{\partial t} = -u \frac{\partial h}{\partial x} - h \frac{\partial u}{\partial x}$$

where u is the velocity of the fluid, h is the height of the free surface, and g is the acceleration of gravity. We will impose the boundary condition $u = 0$ at $x = 0$ and at $x = L$ for all t, implying also that $\partial h/\partial x = 0$ at $x = 0$, L. We seek solutions for u and h for $0 \leq x \leq L$ subject to some arbitrary initial conditions. In this particular sinple example there is neither forcing nor dissipation. (My own interest in these equations is not so much because they represent shallow water waves, but because they are also a simplification of the barotropic primitive equations useful in meteorological prediction.)

For ease in the subsequent development we choose to transform these partial differential equations to a set of ordinary differential equations. We write

$$u = \sum_{n=1}^{N} U_n \sin \frac{\pi n x}{L}$$

$$h = H_0 + \sum_{n=1}^{N} H_n \cos \frac{\pi n x}{L}$$

where the Fourier coefficients U_n, H_n, are the new dependent variables and H_0 is the constant mean height of the free surface. The partial differential equations are now expressed in the form

$$\frac{dU_n}{dt} = \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ijn} U_i U_j - g b_n H_n \qquad (n=1,\ldots, N)$$

$$\frac{dH_n}{dt} = \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ijn}(U_i H_j + H_i U_j) \qquad (n=1,\ldots, N)$$

where the a_{ijn} and b_n are constant coefficients.

3. THE STOCHASTIC DYNAMIC FORM OF THE MODEL

Now let us consider how we approach this problem when the initial conditions are uncertain. We then treat the parameters, the H_n and U_n, as random variables with a joint probability density that corresponds to our degree of belief that different combinations of values are actually taken on. The joint probability density encapsules all of our knowledge of the state of the system with which we are dealing. This knowledge may be based on previous experience with the system, or it may be based on observations. Epstein and Pitcher (1971) discuss the means by which observations are to be used to define the probability distribution.

The equations that govern the behavior of the system depend only on the actual values of the parameters. In making a prediction, however, we can only extrapolate from our current knowledge, which admits of some degree of uncertainty. The equations that extrapolate in time our knowledge will be different from those that predict the behavior of the (unknown) true system parameters. The form of these equations, making essentially the same assumptions, was derived independently by Tatarskiy (1969) and myself (Epstein, 1969).

The joint probability density that represents our knowledge is defined in terms of its moments, and the prognostic equations that are used are equations for the rates of change of the moments.

The first two moments are

$$\left.\begin{aligned} X_i &= E(U_i) \\ X_{i+N} &= E(H_i) \end{aligned}\right\} \qquad i = 1,\ldots, N$$

$$\sigma_{ij} = \sigma_{ji} = \begin{cases} \operatorname{cov}(U_i U_j) & i,j \leq N \\ \operatorname{cov}(U_i H_{j-N}) & i \leq N,\ j > N \\ \operatorname{cov}(H_{i-j} H_{j-N}) & i,j > N \end{cases}$$

The integrals implied by the expectation and covariance operators are over all possible values of the U's and H's weighted by the appropriate probabilities. One way of interpreting the expectation operator is as an average over an ensemble of all possible initial conditions, with relative frequencies in the ensemble being proportional to the assigned probabilities. Later we will employ the ensemble idea to test and evaluate some of our approximations.

The stochastic dynamic equations are:

$$\frac{dX_n}{dt} = \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ijn}(X_i X_j + \sigma_{ij}) - g b_n X_{n+N} \qquad n=1,\ldots, N$$

$$\frac{dX_{n+N}}{dt} = \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ijn}(X_i X_{j+N} + \sigma_{i,j+N} + X_{i+N} X_j + \sigma_{i+N,j}) \qquad n=1,\ldots, N$$

$$\frac{d\sigma_{nm}}{dt} = \text{double sum of terms of form } \{a_{mij} X_i \sigma_{n,j}\}$$

$$+ \text{ simple sum of terms of form } \{b_n \sigma_{m,n+N}\}$$

The equations for the rates of change of the means are somewhat more complicated than those for the "true" parameters. They involve the variances and covariances. The equations for the rates of change of the covariances are still more complex. They are incomplete as shown in that additional terms, involving third moments, have been omitted. The omission of these terms is a convenient and pragmatic choice for closing what would otherwise be an infinite set of equations. So long as the original differential equations are non-linear, the complete expression for the time derivative of any moment will involve the next high moments.

Before examining the implications of the closure assumption, which is of course a crucial aspect of the procedure, we will look at the nature of stochastic prediction. This is illustrated by a film that has been produced entirely through use of the computer. Fig. 1 is the first frame of the film and illustrates the arbitrary initial conditions chosen for the calculations. This is a representation, at time zero (note the clock) of the expected values of the height of the free surface and of the fluid velocity, and of the uncertainties of these quantities. The bounds are one standard deviation on either side of the expected value.

In this representation the Fourier expansion is truncated at wave number five. Note that the standard deviation of u, as well as u itself, goes to zero at the limits x = 0, L(=300km). Also we have chosen values of the variances of the H_n and of the covariances of the height coefficients so as to make our knowledge of the water level less uncertain near the edges than in the middle of the water body. (The tick marks are drawn for every 3 meters, and 3 m/sec. Since the mean depth of the fluid (H_0) is taken to be 30 m, the

tick marks on the upper graph correspond to units of 0.1 h/H_0. The tick marks on the lower graph are for approximately 0.17 $u/\sqrt{gH_0}$.)

A drawing such as this does not represent adequately all of the information contained even in only knowledge of the means and second moments. For example, the initial correlationsbetween the fields of h and u do not effect the appearance of the graph but would be part of our total knowledge of the second moments. (We have assumed these correlations between h and u are zero initially.) Truncating at wave number five, there are ten expected values, and 55 second moments involved in the statement of initial conditions, but 25 of them are not called upon to produce graphs such as shown in Fig. 1.

Fig. 2 presents a sequence of stochastic forecasts (actually individual frames from the film) at 2-hr intervals. One can perceive the basic seiche-like motion that one would expect from the physical analog of our equations. Even the zones of relative certainty and uncertainty propogate back and forth with time. At certain times and places the uncertainty in very substantial, but other aspects of the prediction can be stated with very substantial confidence.

On the whole the uncertainty increases with time. Yet there is a large qualitative difference between the uncertainty initially and after 8 or 10 hours. The details of the shorter waves seem to disappear from the curve for the expected values and instead show up quite strongly in the standard deviations. Indeed, as will be demonstrated more clearly below, the shortest waves rapidly become unpredictable,

especially in the sense that they are advected by an uncertain amount by the flows associated with longer waves. After some time one is still aware that the shorter waves are present, but one cannot be sure where they are located.

4. CLOSURE

The critical aspect of the validity of these predictions is the influence of the closure approximation. In a sense our closure is very similar to the discredited quasi-normal approximation of turbulence theory. In the quasi-normal approximation one evaluates fourth moments in terms of second moments, as they would be related if the distribution were normal. However, one calculates third moments as a significant result and non-zero third moments are inconsistent with the assumed normal relationship between second and fourth moments. The result is internal inconsistencies and calculated turbulent energies that may become negative (cf. Fleming, 1970).

In our closure there are no internal inconsistencies of this nature. Given any set of first and second moments as used in the calculations, there must exist realizable distributions having zero third moments. Thus at each step we are calculating changes for situations which could be real.

The energy of the system is, however, an important aspect of the calculations to examine to seek out any difficulties. In the present model we can usefully define two forms of energy: potential and kinetic, written as

$$PE = \frac{1}{2}\int_0^L gh^2 dx = \frac{g}{2}\cdot\frac{1}{8}(H_0^2 + \frac{1}{2}\sum_{n=1}^{N} H_n^2)$$

$$KE = \frac{1}{2}\int_0^L hu^2 dx$$

$$= \frac{1}{4} H_0 \sum_{n=1}^{N} U_n^2 + \frac{1}{8} \sum_{n=1}^{N} H_n \left(\sum_{n=1}^{N-n} U_m U_{m+n} + \sum_{m=n+1}^{N} U_m U_{m-n} + \sum_{m=1}^{n-1} U_m U_{n-m} \right)$$

The original differential equations, and also the truncated spectral form of the equations require that the sum PE + KE be conserved. Note that the potential energy is of second degree, but that the kinetic energy contains terms of the third degree. The second-degree terms are amenable to representation in the form of spectra; the triple products cannot be so easily represented, but in this calculation (and other applications that we have examined) tend to be small although not entirely negligible.

In stochastic form the energetics are more complex. It is natural to separate the energy into "certain" components, depending only on expected values of the parameters, and "uncertain" components which depend on covariances. We write the stochastic form of the potential energy as

$$PE = CPE + UPE + PE_{min}$$

where

$$PE_{min} = \frac{g}{16} H_0^2 = \text{(constant)}$$

$$CPE = \frac{g}{32} \sum_{n=N+1}^{2N} X_n^2$$

$$UPE = \frac{q}{32} \sum_{n=N+1}^{2N} \sigma_{nn}$$

The kinetic energy is more complex.

$$KE = CKE_2 + UKE_2 + CKE_3 + UKE_3$$

$$CKE_2 = \frac{H_0}{4} \sum_{n=1}^{N} n^2$$

$$UKE_2 = \frac{H_0}{4} \sum_{n=1}^{N} \sigma_{nn}$$

$$CKE_3 = \frac{1}{8} \sum_{n=1}^{N} X_{m+N} \left(\sum_{n=1}^{N-m} X_m X_{m+n} + \sum_{m=n+1}^{N} X_m X_{m-n} + \sum_{m=1}^{n-1} X_m X_{n-m} \right)$$

$$UKE_3 = \frac{1}{8} \sum_{n=1}^{N} \left[\sum_{m=1}^{N-m} (X_{N+n}\sigma_{m,m+n} + X_m\sigma_{N+n,m+n} + X_{m+n}\sigma_{m,N+n}) \right.$$

$$+ \sum_{m=n+1}^{N} (X_{n+N}\sigma_{m,m-n} + X_m\sigma_{n+N,m-n} + X_{m-n}\sigma_{n+N,m})$$

$$\left. + \sum_{m=1}^{n-1} (X_{n+N}\sigma_{m,n-m} + X_m\sigma_{n+N,n-m} + X_{n-m}\sigma_{m,n+N}) \right]$$

$$+ \text{ third moments}$$

To better appreciate this distinction among "certain" and "uncertain" components of the energy, consider a Monte

Carlo experiment in which a large number of calculations are made based on the deterministic equations. Each calculation follows the behavior of one member of the ensemble of possible initial states. Collectively, the results of all of the Monte Carlo experiment give us the answer we seek by the stochastic dynamic equations. Since for each realization the sum of the energies is conserved, the average energy is conserved. But the average energy is the sum of terms that depend only on the average parameter values, plus others that depend on the average values of products of two or three terms that are departures from averages. We will examine the second degree terms only, realizing that their sum is not exactly conserved. (But they are 99-100% of the total energy and are easily shown graphically.) Fig. 3 shows KE, PE and PE + KE, according to whether certain or uncertain. These are based on Monte Carlo sample size of 250, assuming an initial Gausian distribution.

We see several gross features immediately. Looking at the certain components we can discern the normal exchange of kinetic and potential energy. The basic period of this exchange is $L/\sqrt{gH_0}$ or about 290 min. The presence of short waves gives rise to higher frequency modes for the energy.

We also see here the gradual growth of the uncertain energy component and decrease of the total certain energy. The total energy, as shown here, is almost exactly conserved. The missing third order term could not be readily discerned on the scale of this chart.

Calculations of the energies based on the stochastic dynamic equations are shown in Fig. 4. These were carried out for a longer period of time. The Monte Carlo calculations are much more time consuming (by a factor of about 10).

For the period in which the two calculations may be compared the differences are very small, and never greater than what might be attributed to sampling errors of the Monte Carlo experiment.

Note how the higher frequency variations in the certain forms of the energy damp out - but show up increasingly in the uncertain forms. This was an effect also apparent in Fig. 2. After two hundred minutes the total uncertain energy is substantially more than half the certain energy.

In the stochastic dynamic calculations the closure approximation means that there are terms, specifically the third moments, in the energy that cannot be calculated. In other words the energetics which the stochastic dynamic calculations can represent are artifically truncated. Still the stochastic equations will conserve the truncated form of the total energy, so there is no gross inconsistency that will arise.

Further scrutiny of the equations that describe the rates of change of the various energy components points out that the most direct consequence of the closure approximation is that one cannot calculate the non-linear interactions by which uncertain energy is transferred from one wave number to another. This suggests that the first place in which the stochastic calculations will break down will be in the spectral distribution of the uncertain energy.

In figures 5, 6 and 7 we portray the spectral distribution of the energy: potential, kinetic and total; certain and uncertain. Fig. 5 shows this distribution as calculated on the basis of the Monte Carlo experiment; it is shown in Figs. 6 and 7 as calculated by the stochastic dynamic equations. Figures 5 and 6 are almost indescernable from

one another. Even if they are superimposed on one another, the differences are difficult to find. We have made the necessary calculations and therefore know that the numerical value of the terms that are excluded by the closure approximation are of the order of 10%, for this experiment, of the correct values of the derivatives. Remarkable, it would seem, these substantial approximations do not tend to accumulate any substantial imbalances in the spectra of the uncertain components, at least as far as the first eight time steps.

The stochastic spectral calculations are given out to the 200th time step in Fig. 7. Note in particular that the energy in the higher wave numbers becomes almost entirely uncertain. We have good reason to believe that there are still waves of these frequencies present but we do not know where they are. This is the essence of the loss of predictability in meteorological forecasts. The problem is less one of knowing the waves are present, and more of knowing where they are.

It is the particular value of stochastic forecasts what they can quantitatively account for and specify what is predictable and what is not, when it is predictable and when it is not, and just how good any prediction really is.

References

Epstein, E. S., 1969: Stochastic Dynamic Prediction, Tellus, 21, 739-759.

_____ and E. Pitcher, 1972: Stochastic Analysis of Meteorological Fields, J. Atm. Sci., 29(2), to be published.

Fleming, R. J., 1970: Concepts and implications of stochastic dynamic prediction. NCAR Cooperative Thesis No. 22, The University of Michigan and Laboratory of Atmospheric Science, NCAR, 171 pp.

Titarskiy, V. I., 1969: Use of dynamic equations in the probability prediction of the pressure field, Itzvestia Atmospheric and Oceanic Physics, 5(3), 293-297.

Acknowledgments

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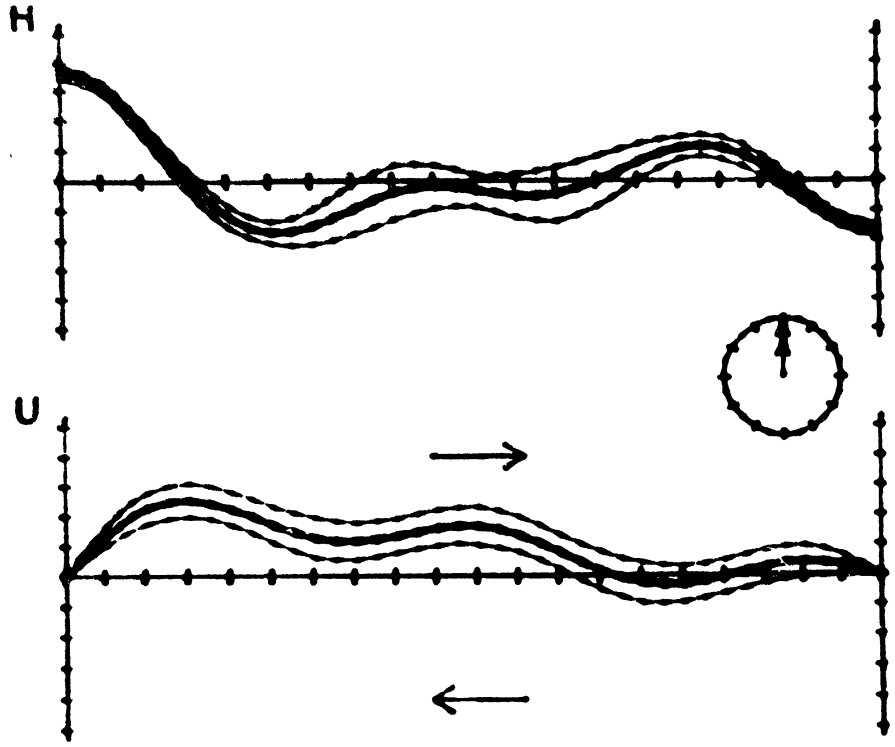

Fig. 1. Initital conditions for the stochastic calculations.

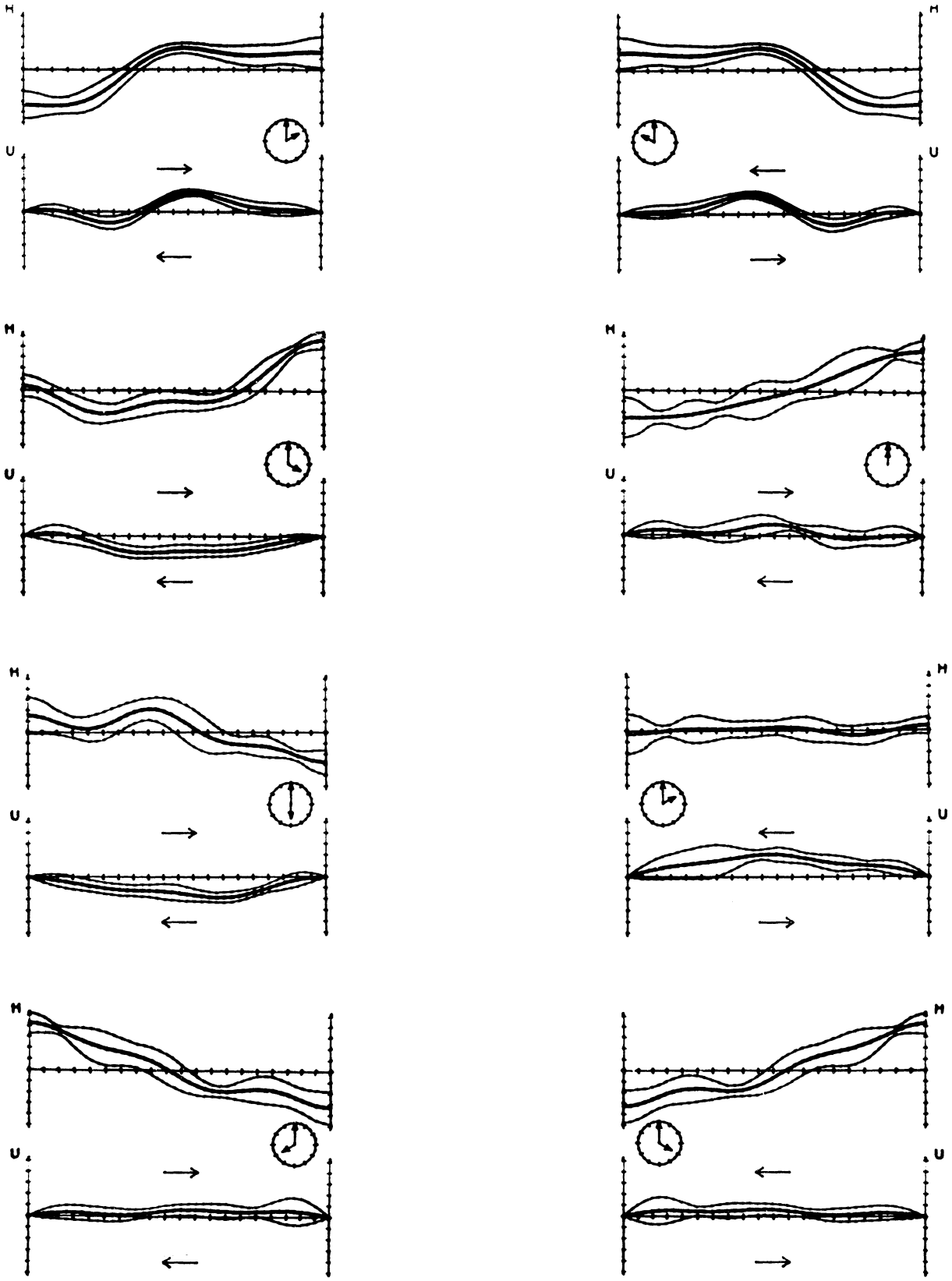

Fig. 2. Sequence of stochastic predictions of the height of the surface and the fluid velocity.

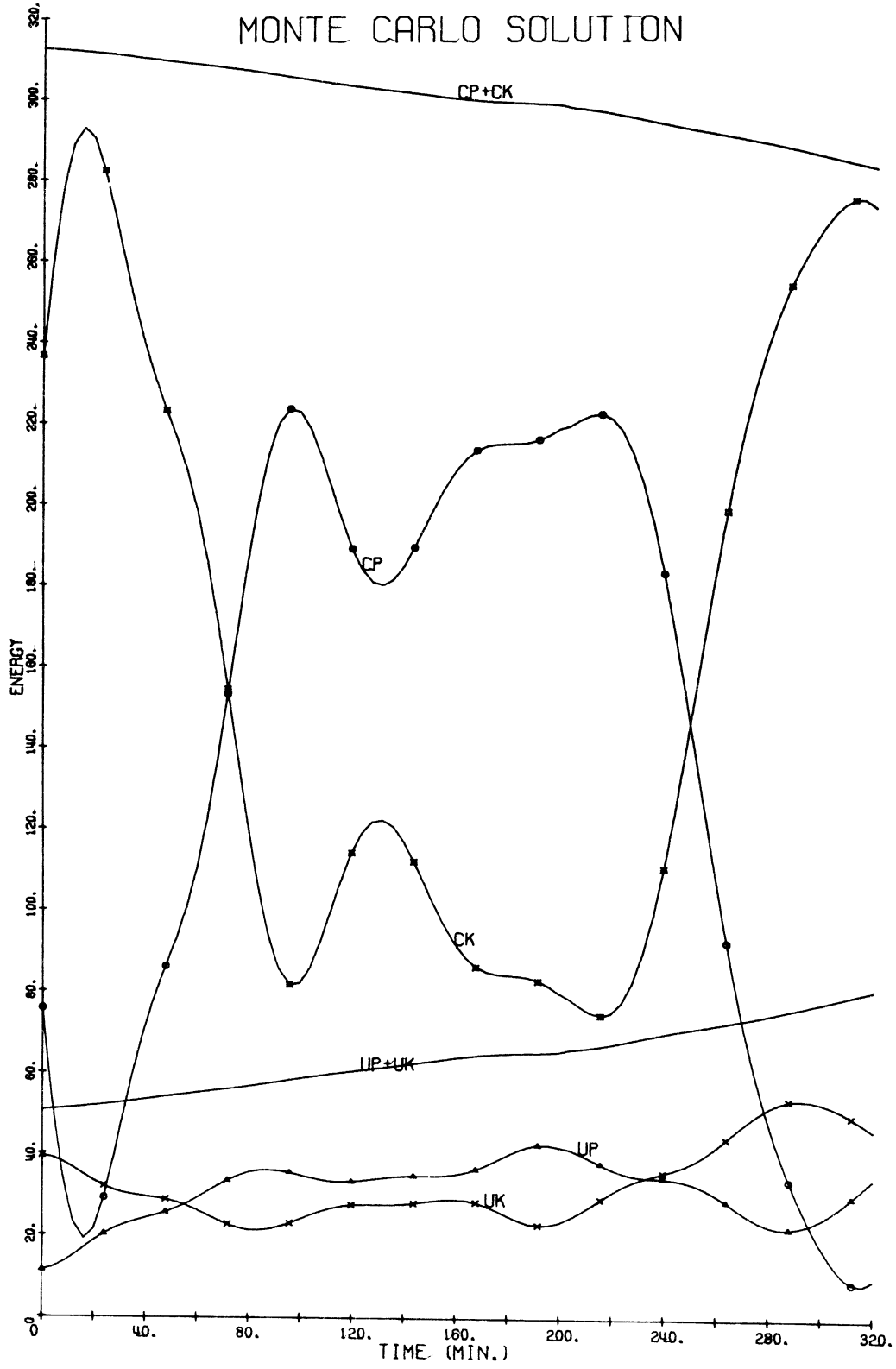

Fig. 3. Energy amounts for the Monte Carlo calculation.

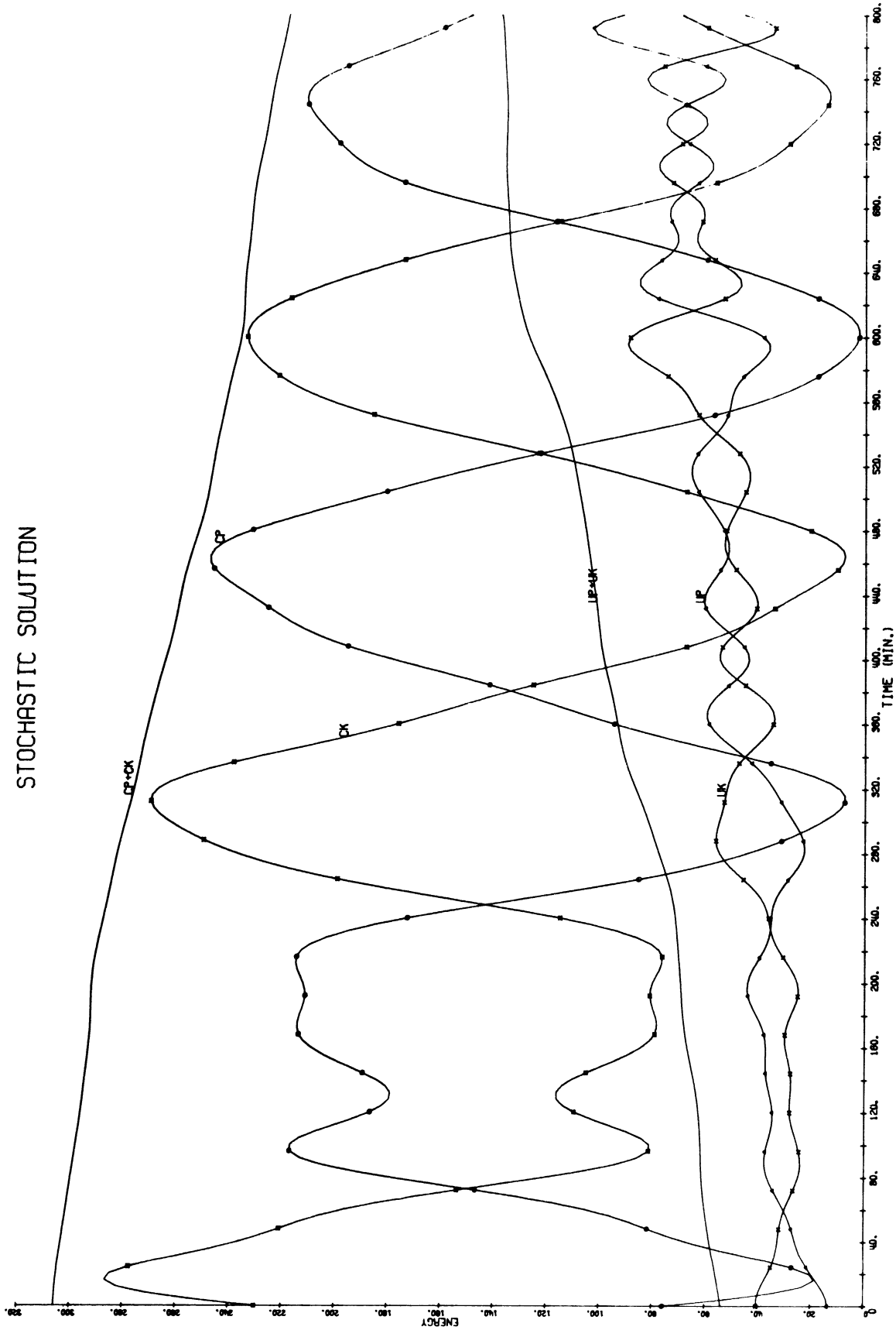

Fig. 4. Energy amounts for the stochastic dynamic calculation.

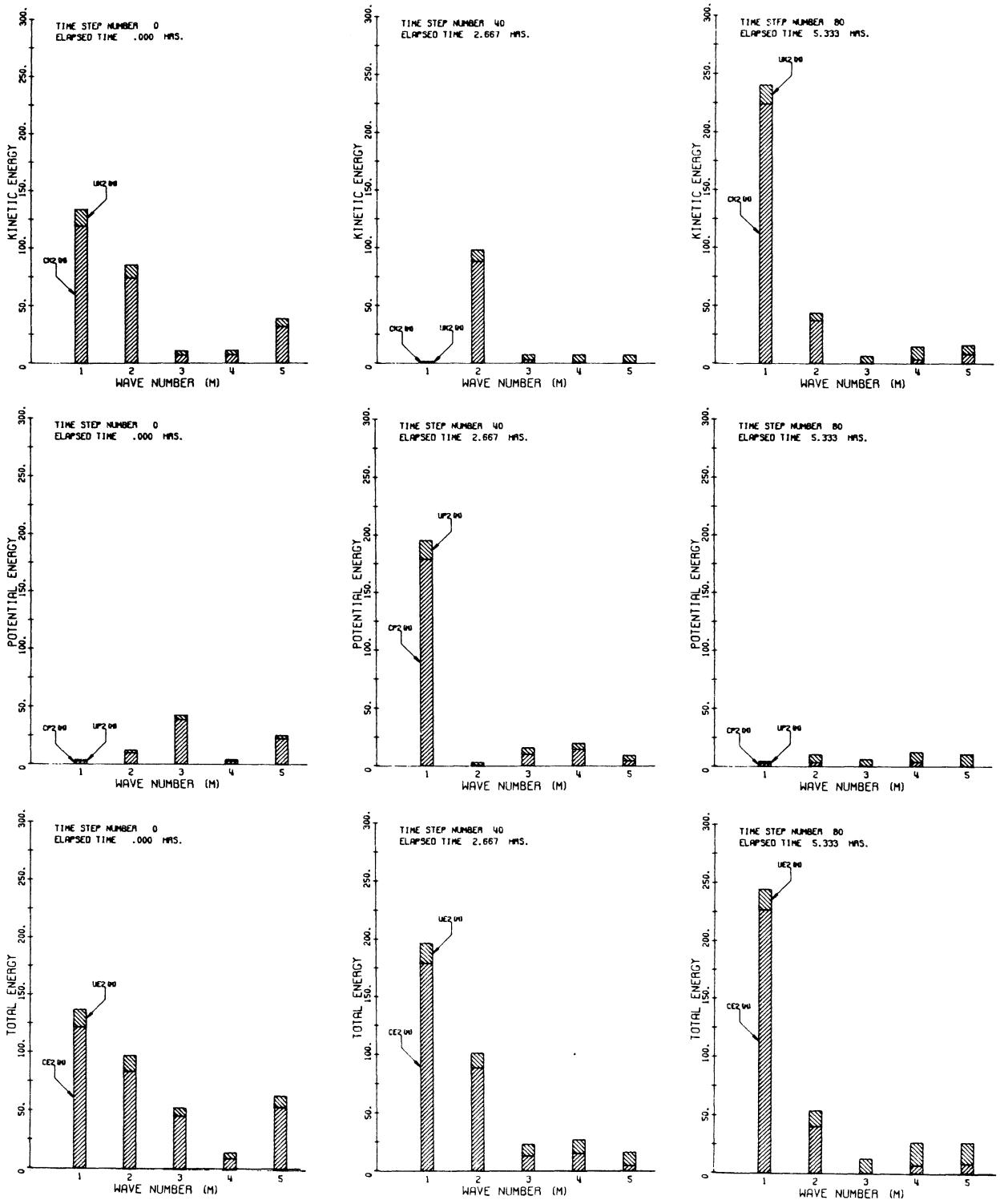

Fig. 5. Energy spectra at three different times for the Monte Carlo experiment. In the top row are the spectra of kinetic energy, the middle row the potential energy, and the bottom row the total energy. Energy that must be represented spectrally as triple product is excluded.

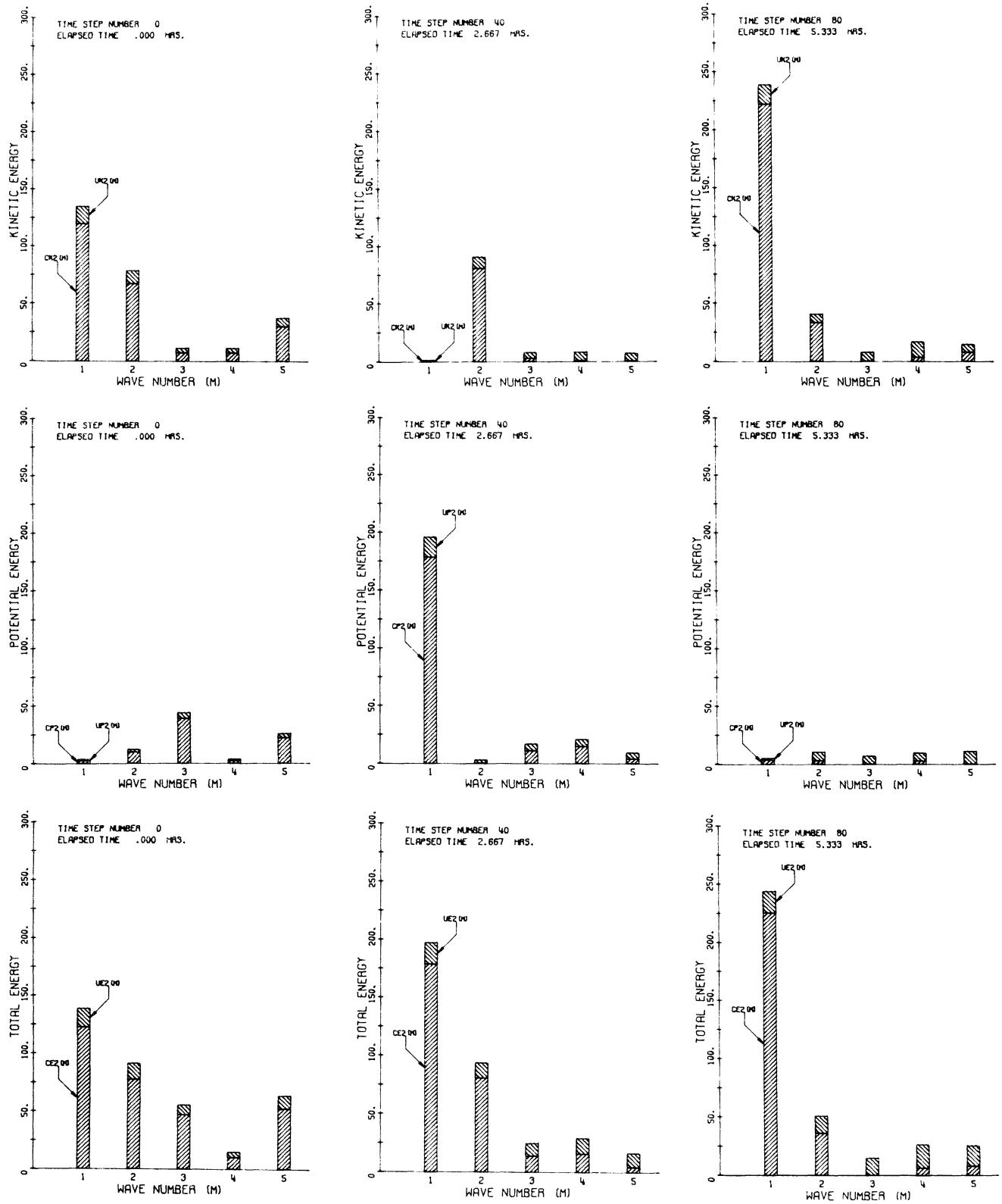

Fig. 6. Energy spectra for the same three times for the stochastic dynamic calculations.

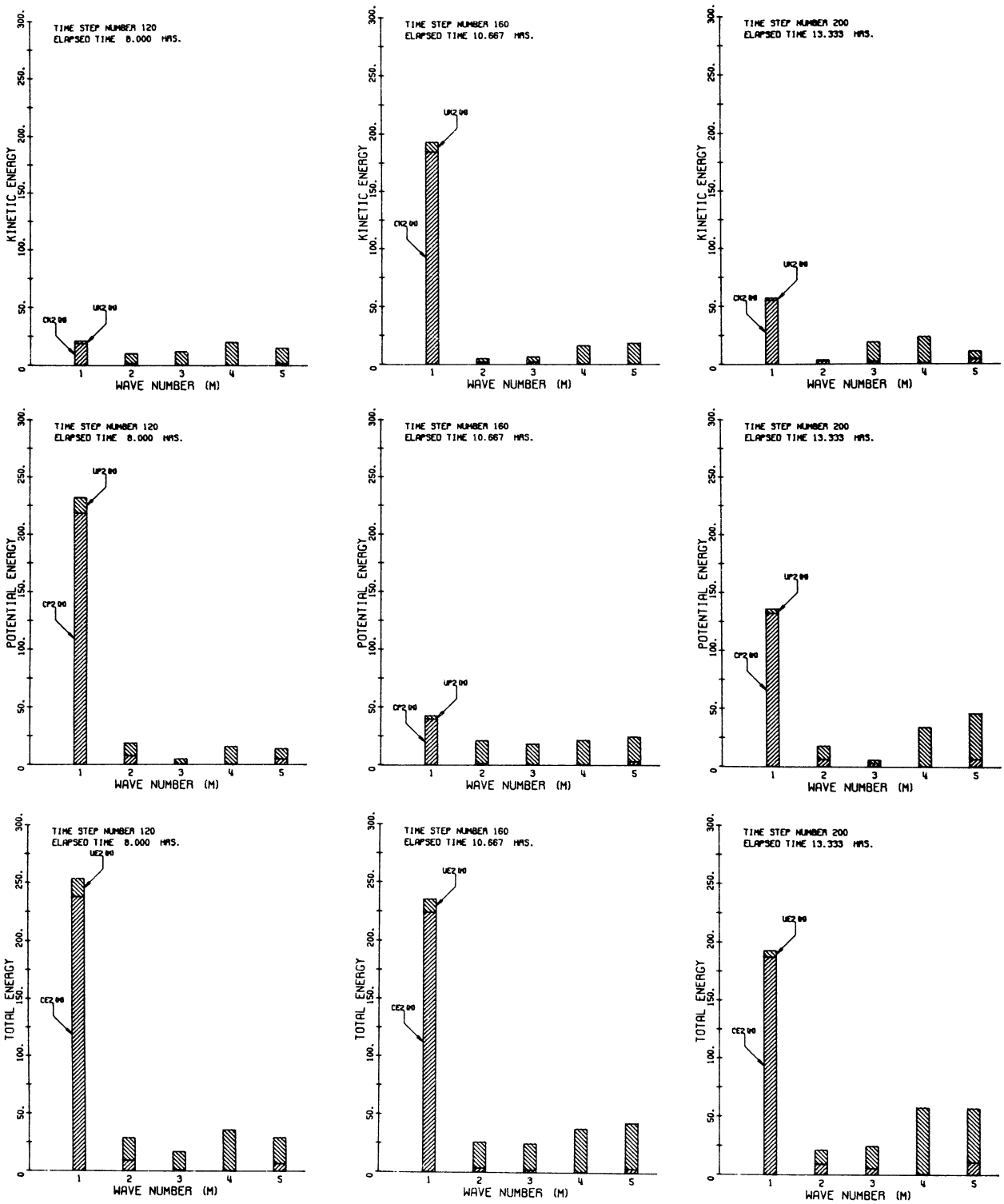

Fig. 7. Energy spectra for the stochastic dynamic calculation after 8, 10-2/3, and 13-1/3 hours.