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Contents

1 Introduction

The WAM model (WAMDI, 1988; Komen et al, 1994) is a so-called third generation ocean wave prediction model. This model integrates the basic equation describing the generation, interaction, propagation and decay of ocean waves. The equation is integrated forward in time on a finite difference grid, with a semi-implicit time integration scheme. Input is a sequence of wind fields (the "forcing wind fields") and if desired an ocean current field. Primary output are the resulting wave fields, characterised by a two-dimensional wave spectrum (frequency and direction) in every grid point, and at every time step within the integration interval. Other wave characteristics such as wave height and direction can be conveniently derived from these wave spectra. The model is widely applied for operational forecasting and for hindcasting, both in global and in regional applications. For a comprehensive description of the model and its field of application, the user is referred to Komen et. al. 1994. A concise description is given in Section 2 of the present report.
Wave observations are available from many sources. There are visual observations from ships, in-situ-measurements from buoys and other platforms. Remote sensing from satellites has become increasingly important. In some cases, only the significant wave height is measured. In other cases (directional buoys, synthetic aperture radar) the full two-dimensional wave spectrum is determined.
Model simulations and observations are complementary. Observations can be used to validate models, and models can be used to extrapolate observations in space and time. In a formal stochastic approach the system is described by a stochastic vector in high-dimensional space. Both measurements and model simulations are realisations of this state and the question then arises how one may obtain the best estimate of the system on the basis of all available information. The process of obtaining this best estimate is called data-assimilation (for the application to ocean waves see Komen et al, 1994, chapter 6).
In practice, one tries to minimise some prescribed cost function, representing a trade off between a number of competing requirements. The minimisation is done with respect to so-called control variables. The specific choice of control variables depends on the nature of the problem one is considering. Typical choices for the control variables are 1. the initial state; 2. a selection of model parameters; and 3. the forcing wind fields. Combinations are also possible. Efficient minimising routines require knowledge of the gradient of the cost function with respect to the control variables.
Another related application, is formed by sensitivity studies. Here also a cost function is defined. One then is typically interested which locations (in space and time) of the forcing fields give rise to the largest sensitivity to the cost function. It may be clear that for this application the gradient of the cost function with respect to the forcing fields is also essential.
So for more than one reason the gradient of the cost with respect to some set of control variables is often required. A complication in calculating these gradients directly is that one needs to take care of the fact that different states (here a wave field) are dependent through the model equations. Therefore, as an alternative, one could calculate the gradient by approximating it by finite differences. The problem,

however, is, that the gradient with respect to each control variable requires an extra model run. So when the number of control variables is large, which is usually the case when initial fields or driving fields are used as control variables, this 'brute force' method is impossible.
A powerful method for handling the model constraints is based on the use of the adjoint model, because it can trace back dependencies in a very efficient way, while taking account of the model constraints. One only needs one adjoint run, which is performed in the opposite direction (usually time) than the model run, to build the information of the gradient of the cost with respect to any input variable, which may be the initial state, forcing fields or model constants. This is in contrast to the finite difference method, where in one run the sensitivity to any output parameter (of which one of them is the cost) with respect to the change in one input parameter is calculated. The adjoint method is therefore *the* instrument to be used in data assimilation. It is superior to sequential methods such as optimal interpolation which consider information at one time step.
Adjoint methods have been applied in different fields, notably in weather prediction (Talagrand and Courtier, 1987; Courtier and Talagrand, 1987). An introduction of adjoint models and a summary of recent advances in the construction of adjoint wave models as well as their their applications may be found in Komen et. al. 1994, which discusses work performed by de las Heras (1992, 1994), Monbaliu (1992a, 1992b), Barzel and Long (1994). and de Valk and Calkoen (1989).
One practical draw back of the adjoint method is that the adjoint model has to be first constructed from the forward model. This can be rather tedious, especially because each application requires its own adjoint. Another complication is that the adjoint model needs all nonlinearities of the model. The problem is that the adjoint model and forward model run in opposite direction. Therefore, first a complete forward model run has to be performed, storing all nonlinearities, which then are used by the adjoint, running backwards. The bookkeeping of the storage and restorage can become very complex.
Recently, a major step forward in adjoint code generation was made by Giering (1995) who constructed an adjoint model compiler (AMC). This compiler is able to directly convert a numerical code into the code for the adjoint problem by regarding the computer source code as the model, which can be adjoined line by line. The automatic adjoint generation is very fast (much faster than compiling the source codes to an executable), which therefore makes the adjoint construction for each application feasible. Another strong point of the AMC is that it takes care of the bookkeeping of the storing and restoring of the nonlinearities.
This report describes the construction of the adjoint of the WAM model with help of the AMC. It is written for those who would like to use the adjoint of the WAM model. A concise description of the physics behind WAM is given in Section 2. In section 3 a short description of the organisation of the WAM code is presented. In section 4, the steps that were necessary to enable the automatic adjoint code generation will be discussed. The structure of the result, ADWAM, will be explained in Section 5. The practical part of this manual starts at Section 6. Here the installation of the updated WAM code, WamC5, will be described, while in Section 7 it is demonstrated how to use the system and how to make the modifications that are needed to adapt the system to the users' requirements.

2 Concise Model Description

In this section we present a basic description of the WAM physics. A comprehensive description may be found in Komen et. al. 1994, or in WAMDI 1988. Going from WamC4 to the present cycle, the physics of the sources has remained unchanged. However, some modifications in the integration method of these sources have been made. These will be described in Section 2.2.

2.1 Model Physics and Dynamics.

The WAM model describes the evolution of a two-dimensional (frequency and direction) ocean wave spectrum. In contrast to first and second generation models, the third generation model WAM introduces no ad hoc assumptions on the spectral shape. It computes the 2-d wave variance spectrum (F) through integration of the transport equation:

$$\frac{dF}{dt} + \frac{\partial}{\partial\phi}\left(\dot{\phi}F\right) + \frac{\partial}{\partial\lambda}\left(\dot{\lambda}F\right) + \frac{\partial}{\partial\theta}\left(\dot{\theta}F\right) = S, \tag{1}$$

where:

F	represents the spectral density with respect to $(f, \theta, \phi, \lambda)$
f	denotes the frequency of the wave
θ	denotes the direction in which the wave propagates
ϕ	latitude of the spectrum
λ	longitude of the spectrum.

The quantities $\dot{\phi}$, $\dot{\lambda}$ and $\dot{\theta}$ denote the rate of change of the position (ϕ, λ) and propagation direction θ of a wave packet travelling along a great circle path.
The source function S is represented as a superposition of the wind input S_{in}, nonlinear transfer S_{nl}, white-capping dissipation S_{dis} and bottom dissipation S_{bot}

$$S = S_{\text{in}} + S_{\text{nl}} + S_{\text{dis}} + S_{\text{bot}}. \tag{2}$$

No change in the source terms from cycle 4 to cycle 5 was made.
The source functions contain several model constants. In the WAM code the values of these constants are equal to those defined in the description of the source terms given below.

2.1.1 The wind input

Ocean waves are generated by wind. This process is quantified by the wind input S_{in}.
The wind input term was adopted from Snyder et. al. 1981 with a scaling with friction velocity u_*. The wind input and dissipation (see Section 2.1.2) terms are based on Janssen's quasi-linear theory of wind-wave generation (Janssen 1989, 1991). The source term has the form:

$$S_{\text{in}} = \gamma \cdot F, \tag{3}$$

The growth rate γ of the waves depends on the friction velocity u_*, and the roughness length z_0:

$$\frac{\gamma}{\omega} = \epsilon\beta(u_*, z_0)x^2, \tag{4}$$

with

$$x = \frac{u_*}{c}cos(\theta - \phi), \tag{5}$$

and where $\epsilon = \rho_{\text{air}}/\rho_{\text{water}} = 1.225 \times 10^{-3}$ is the ratio of the densities of air and water. Here c is the phase speed of the wave under consideration, ω its angular velocity and $\theta - \phi$ is the angle between the direction in which the wave propagates and the wind direction. The details of the relation between β and u_* and z_0, besides a normalising factor β_m=1.2, may be found in Janssen 1991 or Komen et. al. 1994.
In practice, the model is driven with winds at a reference height (usually 10 m). From U_{10} first the friction velocity and roughness length are to be deduced.
According to Janssen's theory, the stress of air flow over sea waves depends also on the sea state and from a consideration of the momentum balance it is found that the kinematic stress $\tau = u_*^2$ is given by:

$$\tau = \left(\frac{\kappa U(L)}{\ln(L/z_0)}\right)^2 \tag{6}$$

where κ=0.41 is Kármán's constant and

$$z_0 = \frac{\hat{\alpha}\tau}{g\sqrt{1-y}} \ , \ y = \frac{\tau_w}{\tau}. \tag{7}$$

Here, τ_w is the stress induced by gravity waves (the 'wave stress')

$$\tau_{\mathbf{w}} = \frac{2\pi}{\epsilon} g \int df d\theta S_{\text{in}} \mathbf{dk}, \tag{8}$$

so through S_{in} itself τ_w depends on the sea state F. The quantity $\alpha = \hat{\alpha}/\sqrt{1-y}$ can be regarded as a sea-state dependent Charnock constant. In WAM, the value $\hat{\alpha}$=0.01 is used, which for old wind sea appears to correspond to α=0.0185, which is the usual value taken for Charnock's constant.
To summarise: given the sea state F and U_{10}, the wind input can be determined. Because of the implicit character of the equations this determination is rather complex. However, this is only a technical complication.

2.1.2 The white-capping dissipation

When two waves meet, the local steepness can become too high, in which case the waves will break. This can be seen as the appearance of white caps.
The dissipation source term is based on K. Hasselmann 1974 white-capping theory, with a modification made by Janssen 1989. It is given by:

$$S_{\text{dis}} = -\frac{C_{\text{dis}}}{2} < \omega > \left(< k >^2 E\right)^2 \left\{\frac{k}{< k >} + \left(\frac{k}{< k >}\right)^2\right\}. \tag{9}$$

Here $C_{\text{dis}} = 4.5$ is a normalising constant, $\omega = 2\pi f$ is the angular frequency and k is the wave number. The symbol $< \cdot >$ is related to an average over the wave

spectrum F:

$$E = \int\int F(f,\theta)df\,d\theta, \tag{10}$$

$$< X > = E\left(\int\int F(f,\theta)\frac{1}{X}df\,d\theta\right)^{-1}. \tag{11}$$

2.1.3 The nonlinear interaction

In principle the theory of surface waves is nonlinear. However, for small steepnesses a perturbative expansion may be made. To lowest order the theory is linear, with the exception of the lowest order nonlinearities that are represented as an interaction between different waves. The theory for this expansion has been developed by K. Hasselmann 1968. In lowest order it contains an integral over resonating wave-vector quadruplets. A set of four waves forms a quadruplet if the wave vectors and frequencies satisfy the resonance conditions:

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4 \tag{12}$$

$$\omega_1 + \omega_2 = \omega_3 + \omega_4. \tag{13}$$

Because the detailed expressions for this interaction is rather complex, they are not displayed in this manual. They may be found in Komen et. al. (1994). In essence it is given by:

$$S_{\rm nl}(1) = C_{\rm nl} \sum_{\rm quadruplets} C(1,2,3,4)F(2)F(3)F(4), \tag{14}$$

where $C_{\rm nl} = 1$ is a normalising factor, 1, 2, 3 and 4 denotes the individual members of the quadruplets and $C(1,2,3,4)$ denotes a cross-section function.
The fivefold dimensionality of the integral over multiplets for the exact expression of $S_{\rm nl}$ is far too expensive for operational purposes. To overcome this problem, the so-called discrete interaction was developed by S. Hasselmann et. al. 1985. This discrete interaction embodies that only a small subset (but such that the physical process is grasped) of quadruplets is given a non-zero cross section. This approach enabled the feasibility of third-generation wave models.

2.1.4 The bottom dissipation

In case of shallow water, waves will loose energy because they 'feel' the bottom. The bottom dissipation term $S_{\rm bot}$ is given by:

$$S_{\rm bot} = -2\frac{C_{\rm bot}}{g}\frac{k}{\sinh(2kh)}F. \tag{15}$$

Here k is the wave number and h the local depth. The normalising factor $C_{\rm bot}$ may depend on the nature and structure of the sediment. In WAM the JONSWAP value $C_{\rm bot}$=0.038 is used.

2.2 The implicit integration scheme

Going from WamC4 to the present cycle two major changes in the numerical integration scheme have been made. They are described below.

In the WAM model the energy balance of the wave spectrum is determined dynamically up to a high frequency cut-off frequency f_c (in operational applications the frequency range is normally between 0.04 and 0.4 Hz). The high-frequency adjustment time scales are considerably shorter than the evolution time scales of the energy-containing frequency bands near the peak of the spectrum, in which one is mainly interested in modeling applications. Thus in the high-frequency region it is sufficient to determine the quasi-equilibrium level to which the spectrum adjusts in response to the more slowly changing low-frequency waves, rather than the time history of the short time scale adjustment process itself.
The WAM model uses an implicit scheme whose time step is matched to the evolution of the lower frequency waves. For low-frequency waves this integration method yields, essentially, the same results as a simple forward integration scheme (but it is of second order rather than first order), while for high frequencies the method yields the slowly changing quasi-equilibrium spectrum.
The implicit difference equations are given by

$$F_{n+1} = F_n + \Delta t\,((1-\alpha)S_n + \alpha S_{n+1}) \tag{16}$$

where Δt is the time step and the index n refers to the time level. The value of α should be taken between 0 and one.
In WamC4 the choice $\alpha = \frac{1}{2}$ was made. It was found, however, by Hersbach and Janssen (1997) that this value could give rise to some numerical noise in the calculation of the wave stress. When the choice

$$\alpha = 1 \tag{17}$$

is made, these fluctuations are mostly suppressed. Therefore this is the value for α that is used in the present cycle.
Unfortunately, S depends nonlinearly on the spectrum F, hence we cannot solve directly for the spectrum F_{n+1}. Therefore, S_{n+1} is expanded around F_n,

$$S_{n+1} = S_n + \Delta F \frac{\delta S_n}{\delta F} + \cdots \quad , \quad \Delta F = F_{n+1} - F_n, \tag{18}$$

where only the linear terms in ΔF are retained and $\delta S_n/\delta F$ denotes the functional derivative (a matrix in discrete notation). Under the approximation that only the diagonal terms of $\delta S_n/\delta F$ are retained, one can solve directly for F_{n+1}.

2.2.1 The limitation of wave growth

In practice, it turns out that the resulting numerical scheme is not always stable at high frequencies near the model cut-off and, as a safeguard, a limit on the increments of F has been imposed. It was found by Hersbach and Janssen 1997, that the limiter of WamC4 gave rise to incorrect results when using very fine grids and time steps. As a result, the WamC4 model severely underpredicts wave height, when implemented on lakes. This incorrectness has been removed in the present cycle, by introducing an alternative limiter:

$$\Delta F|_{\max} = 3.0 \times 10^{-7} g \tilde{u}_* f^{-4} f_c \Delta t, \tag{19}$$

where $\tilde{u}_* = \max(u_*, g f^*_{\rm PM}/f)$ and $f^*_{\rm PM} = 5.6 \times 10^{-3}$ is the dimensionless Pierson-Moskowitz peak frequency.
The inclusion of a minimum to u_* anticipates windless situations. In this case, the limiter would reduce to zero, which means that swell dissipation would be prohibited.

2.2.2 Initial wave growth

The source term in the WAM model are all quasi-linear, which means that they are all proportional to the wave spectrum. The proportionality factor also depends, in some form, on the wave spectrum. This has the somewhat undesired property that an initial wave-less sea, will remain wave less: no energy can be transformed to the perfectly flat sea surface. In practice, such a situation will never occur. However, it can happen that, due to propagation and/or dissipation, certain parts of the two-dimensional spectrum have zero wave energy. When then suddenly a wind rises in this direction of the spectrum, this should give a quick development of wave energy. However, due to the quasi-linearity, it will take far too much time before this will actually happen. Besides, the early wave generation is a subgrid scale process in WAM. Therefore, initial growth needs to be parametrised. This was achieved by introducing a minimum (nonzero) energy level in the present cycle.

$$F_{\mathrm{MIN}} = 1.0 \times 10^{-12} \frac{g^2}{(2\pi f)^5}. \tag{20}$$

This minimum represents a fraction of a Pierson-Moskowitz spectrum, is isotropic and only represents very little wave energy. However, it will trigger the (fast) wave growth at the high-frequency part of the spectrum in the wind direction.

3 The WAM code

The supervising module of the WAM-ADWAM system is the routine CHIEF. Its flow diagram is given in Fig. 1. Depending on the choice to perform a forward or adjoint run it calls the routines WAVEMDL or ADWAVEMDL. Their flow diagrams are given in Fig. 2. In these routines the actual WAM integration (by calling subroutine WAMODEL, see Fig. 3) and ADWAM integration (by calling subroutine ADWAMODEL, see Fig. 4) are performed.

3.1 The data assimilation part

The main routine of the WAM model is the subroutine WAMODEL:

```
SUBROUTINE WAMODEL(XCONTROL,FC)
```

The flow diagram of the subroutine WAMODEL is given in Fig. 3. As input it requires the set of control variables XCONTROL. First a connection between the control variables and the WAM model is made. This connection is established in the routine XCONNCT. Then the model is integrated in time. During this integration, model results are connected to a cost, which typically represents the misfit between model results and data. The connection between the model results and the cost is defined in subroutine NEWCOST. At the end of the integration the total cost is returned to FC.
If the user wants to adapt the WAM model to its own data assimilation scheme, in principle the only two routines he or she has to modify are the routines XCONNCT (in order to define the appropriate control variables) and the routine NEWCOST (to define the appropriate cost). If the user wants to add a first guess penalty to the cost, the ideal place for this is also routine XCONNCT.
The routines XCONNCT and NEWCOST are both inside the file wam.cpp, which is located in the src/chief directory.

3.2 The model part

The routine WAMODEL integrates the model forward in time. Its flow diagram is given in Fig. 3.
First the model is initialised. The restart spectra and the initial wave stresses are read from file. Also the connection between the control variables and the model is established. These actions take place in the routines INITMDL, XCONNCT and PREWIND.
Next a time loop is performed, in which the wave spectrum is updated step by step. The length of the steps is IDELPRO, the time between two propagation steps. In this loop first the wave field is propagated in routine PROPAGS. Then in subroutine IMPLSCH new forcing wind fields are determined (when necessary), the sources are calculated (see Section 2.1) and finally the sources are integrated on the basis of the implicit scheme discussed in Section 2.2. In addition, the cost is updated. Finally, if desired results are written to output. The time step of the source term integration (IDELT) need not to be equal to IDELPRO. Only the (inverse) ratio should be an integer.
The routines WAMINIT, INBLOCK and OUTSPEC are, amongst other things, concerned with the multi-block version of the model. In the latter routine also a restart spectrum and wind-stress file for the end date of the integration is produced. These can be used as input for a following model run.
The model can be run under various options. These are explained in Section 7.2.5.

4 The construction of ADWAM, using AMC

4.1 Introduction

The AMC constructs an adjoint on the source code level. As input the Fortran 77 code of the model is given, as output the Fortran 77 source code of the adjoint model is returned, as well as a modified forward source. The difference between the original forward code and the modified code is the inclusion of calls to routines (adstore or adwrite) that take care of the storage of the nonlinearities of the model. When such a storage call has been added, in addition at the end of that routine, a routine adcount is included that takes care of the bookkeeping. These storage routines are accompanied by restoring routines in the adjoint code. For a detailed description of the AMC, the user is referred to Giering (1995).
Before the AMC could be successfully applied to the WAM model the code had to be edited at several places. This did not alter the model results. The changes may be categorised in the following classes:

4.2 Inclusion of CADJ directives

First of all the AMC needs specific information, whether a certain variable, common block, or even a complete routine depends on the control variables or not, and whether it influences the value of the cost. Only when both dependencies do occur, such structures need to be adjoined, leading to the construction of an associated adjoint variable, adjoint common block or adjoint routine. This information the user has to handle to the AMC by the inclusion of directives in the source code. These have the form:

```
CADJ VAR              X = CONST
CADJ COMMON      XBLOCK = CONST
CADJ SUBROUTINE    XSUB = CONST
```

where X is a variable, XBLOCK a common block and XSUB a subroutine. A Fortran compiler will ignore such directives. In principle an adjoint compiler should be able to perform an analysis on what should be adjoined (ACTIVE), and what shouldn't (CONST), given the set of control variables and the cost function. Such an analysis is in general very time consuming and delicate and is not handled by the AMC. However, the successor of AMC, the Tangent and Adjoint Model Compiler (TAMC), see Giering 1996, is capable of performing this analysis. In principle the adjoining of structures that are not necessary will not affect the result. However, this could introduce a large number of needless adjoint statements and the storage or recalculations of many irrelevant nonlinearities.
Another form of directive instructs the AMC to add a storage routine that will store a certain nonlinearity. These directives have the form

```
CADJ STORE <VAR> = <AMCDEVICE>
```

where <VAR> represents the nonlinearity to be stored and <AMCDEVICE> indicates whether this will be stored to file (FILE) or memory (MEMORY). In principle the AMC will try to recalculate each nonlinearity if needed in the adjoint code. When it assumes that such a recalculation is not possible, it will produce a warning. The inclusion of a CADJ STORE directive may then be necessary. By the way, the algorithm AMC uses to decide whether a recalculation is possible or not, is not entirely sufficient for arrays. As a result it will sometimes report an unnecessary warning. This is also the case for WAM, where such warnings are reported within the routines PROPAGS, IMPLSCH and WAMODEL.
The inclusion of CADJ directives is not unique. Different inclusions can lead to the same correct adjoint. However, the performance both in space (the number of nonlinearities to be stored) and time (needed to store and restore them) can vary enormously. To optimize time, CADJ STORE directives were put in outer loops as far as possible. In addition they were located at places where they could be used in a as large as possible part of the model. In addition, sometimes it was chosen to recalculate nonlinearities rather than storing them. To allow for this optimisation it was necessary to restructure some routines. As a result about the size of 3.1 restart spectra needed to be stored per time step. The time consumed of this storage is less than 1% of the model run time. ADWAM is about 70% slower than WAM. This performance is quite satisfactory.

4.3 Troublesome Fortran 77 structures

Because the AMC should build an adjoint model running in reverse order, it must be able to disentangle the flow of the model. Fortran 77 structures, such as GOTO and DO WHILE loops make such an analysis very difficult. Therefore they are prohibited by the AMC. In WAM, GOTO statements typically are used to check whether a certain date has been reached. These GOTO's could be circumvented by explicitly calculating the number of times it takes before such a date is reached.
Besides, only ACTIVE routines need to be adjoined. By indicating this with a CADJ directive, or by simply excluding this routine from the input source file, AMC will

not protest against troublesome structures in such routines. Many GOTO's appear in CONSTANT routines.
However, for the wind routines, the complexity introduced by the invokement of GOTO statements made it necessary to rewrite the routines PREWIND, NOTIM and TIMIN completely. In fact, the routines TIMIN and NOTIM have been replaced by a single routine NEWWIND, which takes care of the bookkeeping when to read an external wind field and how to interpolate this (in time and space) to an internal wind field used by the model. The routine PREWIND is only called at the beginning of the WAMODEL run, in order to read the first external wind field. There is no need anymore to store intermediate wind fields to file, as was the case for the previous cycles.

4.4 Smoothing the WAM code

The AMC generates the exact adjoint of the computer source. This forward source code may contain many conditional statements, which may cause localised jumps of the cost in control variable space. The adjoint gives the very local behaviour of the cost, which might not reflect a more global behaviour. A construction of the adjoint code from the equation level will not suffer from this possible inconvenience. This, however, is a very tedious operation. Besides, due to discretisation of the adjoint equations, the resulting adjoint code may not reflect the exact adjoint. One should be aware of the abovementioned and make sure that the model contains as less as possible local discontinuities.
An example of a routine that will give a problem is PEAKFR, which calculates the peak frequency at each grid point. It is not used inside WAM, but it will typically appear in a cost function. In cycle 4 the peak frequency was taken to be the frequency of the bin of the frequency spectrum that has the highest energy density. This number will not change when some control variable will be changed infinitesimally. Therefore the local gradient is zero, which is exactly what ADWAM will produce. Clearly this is not desired, because PEAKFR will produce a cost that is locally flat, but makes many jumps. To remedy this, a parabolic interpolation was made. The resulting peak frequency does continuously depend on the control variables.

4.5 The multi-block version and nested grids

To enable model runs with a large number of grid points on computers with limited memory, the multi-block version of WAM was developed in a previous cycle. The grid is in such a case split into a number of blocks, in which only two blocks at a time need to be present in memory. These blocks are read from and written to the restart file. For the adjoint code this should be accompanied by the reading from and writing to an adjoint restart file. The reading and writing of adjoint variables is a complication AMC cannot handle. In principle this adjoint part could be constructed by hand. However, since the running of an adjoint requires a lot of memory and disk space anyway, it was decided not to do this. Therefore the adjoint code only works for single-block runs. The forward code, still works for both the single and multi-block option.
A way to decrease computing time for a large application is to make use of nested grids. In this case a finer grid uses boundary information generated by a coarser

grid, embracing the fine grid. This also involves the reading and writing of spectra and is therefore also not handled by AMC. So ADWAM will not work correctly for the connection between coarse and fine-grid runs. However, it will produce correct results for the fine run, in which the boundaries, produced by the coarser run, are regarded to be CONSTANT.
The parts of the WAM code that are specifically designed for the multi-block version and nesting should be regarded as CONSTANT to AMC. However, in cycle 4 these parts where inside routines that also contain active parts. Therefore, to make things easier, the constant parts were collected into additional subroutines. Also the model-output part of WAM, which is usually not connected to the cost, was collected in separate routines.

4.6 The flexibility of WAM

When optimising a model, it will usually take a number of iterations to reach a desired degree of satisfaction. Also, because the amount of nonlinearities can become so huge, one sometimes has to split the model run into smaller parts (the check-point method, which will do this, is described in Section 5.2). Both require that it should be made very easy to rerun the model and to run it at earlier dates (necessary for the check-pointing). This required flexibility was not present in WamC4. The restart files, containing the initial spectrum and initial stresses, were overwritten with the final spectra and stresses. The user then first had to copy the restart files to other locations to enable a rerun of the model. Also some files were copied inside the WAM model by invoking system calls, which are computer dependent. To make the WAM system more flexible, restart files are not overwritten anymore, but are labeled with a date.
Special attention was given to the multi-block option. For this the way in which spectra are stored on file was modified. The size of the files has been decreased, and the storage of spectra for overlapping latitudes has become obsolete.
There is one single routine, OPENFIL, that takes care of the fetching of Fortran units to date-labelled files. It is only composed of standard Fortran 77 code. In addition, dates are represented by CHARACTER*10, rather than by INTEGER, as was already the case for the work-station version of WamC4. Therefore the WAM code has become computer independent and should be able to be installed easily on any system containing a Fortran 77 compiler.

4.7 The hiding of code from AMC

At some locations, it was desirable to hide parts of the forward code from AMC. This was established by adding the structure C_AMC at the beginning of such lines. AMC will regard them as comment and constructs the adjoint and modified forward code, as if these lines were not present. Then the modified code is postprocessed by means of a C-preprocessor, telling to remove the C_AMC's. The hidden lines are then recognised by again by the Fortran compiler. There were two occasions for which this somewhat inelegant construction was used.
Most problems regarding GOTO statements could be circumvented. However, some extra care was needed in routine BOUINPT, which reads in boundary information from a coarse grid run. The adjoint of this routine only needs to reset the adjoint variables of the spectra at the boundary. The input boundaries themselves are

CONSTANT variables. Their evaluation, which takes place in the same routine, involves rather troublesome structures for the AMC. This evaluation is irrelevant for ADBOUINPT, and therefore the lines were screened with the inclusion of C_AMC. The modified forward code includes the storage commands. However, when one is only interested in a forward model run (controlled by a variable IADJNT=0), the storage of nonlinearities is obsolete and might prohibit the run because of lack of disk space or memory. Therefore these routines should only be called when the adjoint model is to be run (IADJNT=1). If one simply writes:

```
      IF(IADNT.EQ.1) THEN
CADJ  STORE X = FILE
      ENDIF
```

AMC will still try to recalculate X because if IADJNT.NE.1. it will need the value of X. AMC does not know that the user is only interested in the nonlinearities when IADJNT.EQ.1. This can lead to many complications. The inclusion of C_AMC before the beginning and end of the loop gives precisely the desired result:

```
C_AMC       IF(IADNT.EQ.1) THEN
CADJ  STORE X = FILE
      CONTINUE
C_AMC       ENDIF
```

The CONTINUE statement has been included to prevent that AMC will place the call of the storage routine outside the loop.
Sometimes AMC decides to place the call to adcount after a RETURN command, which will in effect never be accessed and will mix up the bookkeeping. As a third application these RETURN statements could also be hidden with C_AMC. In WAM, the RETURNS typically appear just before the END statement and therefore they could be safely deleted instead.

5 The ADWAM code

The supervising module of the WAM-ADWAM system is the routine CHIEF. Its flow diagram is given in Fig. 1. Depending on the choice to perform a forward or adjoint run it calls the routines WAVEMDL or ADWAVEMDL. Their flow diagrams are given in Fig. 2. In these routines the actual WAM integration (by calling subroutine WAMODEL, see Fig. 3) and ADWAM integration (by calling subroutine ADWAMODEL, see Fig. 4) are performed.

5.1 The general structure

The main routine of the AMC-generated adjoint code is ADWAMODEL:

```
SUBROUTINE ADWAMODEL(XCONTROL,FC,ADXCONTROL,ADFC)
```

Its flow diagram is given in Fig. 4. As input it requires the values of XCONTROL used by the forward model and the resulting cost (These can be regarded as the first required nonlinearities of the model). Also the adjoint variable of the total cost ADFC should be initialised with ADFC=1, all other adjoint variables should be reset to zero. It is exactly at this location where it is decided with respect to

what forward model result the gradients are calculated. If one would have initialised a different adjoint variable to unity and the rest to zero instead, the result of the adjoint run would reflect the gradients with respect to its corresponding forward variable.
Next the adjoint model is integrated in the reverse order in which the forward model has been integrated. Each active statement of routine is reflected by a corresponding adjoint statement. The results of IF statements have been stored during the forward run (they can be regarded as a severe form of nonlinearities). They are restored in the adjoint run, so that the adjoint can trace back the precise tree structure of the forward model run.

5.2 Check points

As was already stated in the previous section, each integration time step the amount of nonlinearities to be stored adds up to the size of three restart spectra. For realistic applications this can add up to enormous numbers. For instance, for a hindcast of several days in the North sea, regarding the resolution used at KNMI, each restart file has a size of about 3.8 Mbyte. A five-day run, using a time step of 600 s, would add up to 8 Gbyte of required disk space. To avoid storage problems, a 'check point' method has been implemented. First the five-day run is chopped into smaller WAM runs of each three hours. At the end of each smaller run a restart file is dumped. Only for the last three-hour run the nonlinearities are stored. Then ADWAM can be run from the end date up to three hours earlier. Next on the basis of a restart file saved during the chopped forward run, the one but last three-hour run is rerun and overwrites the previously stored nonlinearities. Then ADWAM can be run another three hours backwards. This recipe is repeated until the adjoint hits the start date. The benefit is the enormous saving of disk space: now 'only' 350 Mbyte of disk space is required, which is a feasible size. The drawback of the check point method is that one effectively has to perform an extra forward run in order to complete an adjoint run. So WAM+ADWAM, now will require the time of 3.7 WAM runs, instead of 2.7 which would be needed without the check pointing. Clearly the saving in disk space surpasses the extra involved computational burden considerably. In this example we made a choice of a three-hourly check pointing. In general one can show that the optimal check-pointing interval (in units of time steps) is given by $n_{\rm opt} = \sqrt{N/a}$, where N is the total number of time steps and a is the required disk space per time step in units of restart spectra (a=3 in the present case). The reduction in required disk space is a factor $\frac{1}{2}\sqrt{aN}$. This optimum, however, is quite broad, which admits a deviation from $n_{\rm OPT}$ that meets the practical situation.
The check-point method has been implemented in the WAM-ADWAM system, by constructing a supervising routine that calls WAMODEL and ADWAMODEL in the correct order. For both the forward model as for the adjoint model such a routine was constructed. Their flow diagrams are given in Fig. 3.
Subroutine WAVEMDL chops the forward integration into little WAMODEL runs, of each one check-point integration time long. It ensures that the nonlinearities are overwritten each WAMODEL run.
Subroutine ADWAVEMDL performs the actual check pointing. First it performs a forward integration over the total integration time. Then it initialises the adjoint variables. Next WAMODEL and ADWAMODEL are called repeatedly for the correct integration periods. At the end it returns the gradient with respect to the

cost.

5.3 Possible complications

As was already indicated in Section 4.4, ADWAM is the adjoint of WAM on the source code level. Therefore it will inherent the numerical noise of WAM. This can be a serious problem, because the gradient calculated by ADWAM only describes the very local behaviour of the model. Generated by the numerous IF statements, this local behaviour might be quite different from the more desired global behaviour of the model. Our experience is that this complications were sometimes a problem, and in other cases not. The user should therefore always be very careful. For instance, when one compares model results with data, on could average the model results over a small time and space domain, rather then just taking the value of the model result at the exact location and time. In this way, the local jumping of the gradient will be reduced.
It is very difficult to find the locations in the WAM model which can give rise to the noisiness of the model. So, once again, the user should be careful and test his or her system thoroughly.

6 Installation of the WAM system

The actions described below can also be found in the README file.
The WAM system, as presented here, consists of the following modules:

- The PREPROC module, which is used to precalculate time-independent quantities, such as reading in the bathymetry, constructing shallow water tables etc.
- The PRESET module, which is only to be used to produce an initial wave spectrum, as input for a cold-start WAM model run.
- The CHIEF module, which contains the actual WAM model integration part and the ADWAM integration.
- The AMC module, which is used to construct ADWAM from WAM. It contains the library in which the routines for the storage and restorage of nonlinearities are defined.

In this section we will describe how to install these modules. The installation is based on a grid in the North Sea. To keep things as simple as possible, artificial wind fields, artificial control variables and an artificial cost function is used. However, these will grasp the essence of adjoint modelling. In section 7.2 it is explained how the user can adopt the system to his or her application.
The WamC5.tar.Z file contains the complete WamC5 model, including the AMC. To install the system, perform the following steps:

- uncompress the WamC5.tar.Z file:

```
uncompress WamC5.tar.Z
```

  The file should be transformed to WamC5.tar.

- Untar the file:

```
tar xvf WamC5.tar
```

  As a result the WamC5 directory should be created.

- Installation of AMC. This step is only necessary when the user has the intention to use ADWAM.
  in the directory WamC5, there is a subdirectory amc_3.97. Enter this directory. Then copy the Make.host.<your machine> to the Make.host file. So if you for instance intend to install the system on a SUN work station type:

```
cd WamC5/amc_3.94
cp Make.host.sun  Make.host
```

  The amc is installed by typing:

```
make install
```

  The AMC executable will be constructed, as well as the AMC library libamc. If the make command fails it does not mean that the AMC executable and library have not been constructed. The user can check this by typing:

```
amc -help
```

  If a AMC header appears followed by an option list, the AMC part of the installation has been successful.

- Construction of the PREPROC executable.
  In the WamC5 directory there is a src/preproc directory. This directory contains the files: preproc.cpp, preproc.f and makefile.

  The file makefile contains the instructions to compile the preproc module, which is described below. This makefile is just a very basic one. The user may find it appropriate to refine it for convenience. It performs the following two steps:

  First the preproc.cpp file is preprocessed using the cpp command. The result is the preproc.f file (which is already present in our case). It may be necessary to include the full path of the command cpp, in which case /bin/cpp is a good guess.

  Next makefile will compile the module, which should result into the preproc.exe executable, which is located in the bin directory of WamC5. It is assumed that the command for the invokement of the Fortran compiler is f77. If this is not true, the user will have to adapt this.

  The makefile is executed by:

```
cd ../src/preproc
make
```

- Construction of the PRESET executable.
  The same instructions as for PREPROC apply, i.e. replacing preproc by preset:

```
cd ../preset
make
```

- Construction of the CHIEF executable.
  the src/chief directory contains two .cpp files: wam.cpp and const.cpp. The first file contains the routines that are important for the construction of ADWAM. The const.cpp contains the CONSTANT routines and the top level routines CHIEF, WAVEMDL and ADWAVEMDL that control the WAM-ADWAM system.

  The file makefile controls the construction of ADWAM.

  Before ADWAM can be constructed, first AMC has to be installed (see above). The makefile will first preprocess the wam.cpp and const.cpp files to the files tmp/pre and const.f respectively. Then, it will invoke AMC on tmp/pre, which will result in a modified forward code tmp/pre.f and an adjoint code tmp/pre_ad.f. Next the tmp/pre.f will be postprocessed (i.e. removing all C_AMC comments discussed in Section 4.7) to wam.f. The file tmp/pre_ad.f is copied to adwam.f. Finally const.f, wam.f and adwam.f are linked to an executable chief.exe, which is located in the bin directory of WamC5. AMC will create a logfile amc.log, reporting about the status of the constructed adjoint code. In our case the logfile is already present, which may be used as a reference. This is all achieved by typing:

```
cd ../chief
make
```

  If the user is only interested in running the forward model and not ADWAM, he or she should do the following:
  Remove the call to ADWAVEMDL in subroutine CHIEF, and the CALL ADMZERO in subroutine WAVEMDL. Both can be found in the file const.cpp.
  Run the constant.mk file:

```
cd ../chief
make -f constant.mk
```

7 How to run the WAM-ADWAM system

The actions described below can also be found in the README file.

7.1 The test run

Now AMC, its library and the executables preproc.exe, preset.exe and chief.exe have been installed, the test run can be performed. For this enter the jobs directory of WamC5. Here, three jobs, preproc.job, preset.job and chief.job are present. The jobs run the *.exe programs. As input the so-called user input files in the subdirectory

input are presented to these executables, the output generated by the executables are redirected to logfiles in the subdirectory output. Binary output files, such as restart spectra will be stored in the WamC5/restarts directory.
First execute preproc.job to generate time-independent quantities. As input it reads the input/preproc file and the units fort.1 and fort.2. They are linked to the bathymetry file WamC5/grids/topocat and WamC5/grids/curcat. The result should be:

- An ascii output file output/preproc.
- Two binary files in WamC5/restarts: PRECOMMO_UBUF which contains the neighbour indices of each grid point and PRECOM_BLOCKS which contains other time-independent quantities.

Next execute preset.job to generate a first restart spectrum. In this case this will be for February 2, 00h00m 1991.
Preset.exe will use the PRECOMMO_UBUF and PRECOM_BLOCKS files generated by preproc.exe. The result should be:

- An ascii output file output/preset.
- Two binary files in WamC5/restarts: RSS9102020000 containing the restart spectrum, and RSW9102020000, containing the wind field interpolated to the WAM grid and the wave stress.

Finally execute chief.job to perform a combined WAM-ADWAM run, in this case from February 2, 00h00m 1991 to February 2, 02h00m 1991. First a forward model run is performed to store the nonlinearities of the model and the cost. Then the adjoint is run to calculate the gradient of the cost with respect to the control variables. Finally, a number of forward model runs, each with a slightly different setting of control variables are performed, in order to check the gradient by 'brute force' is integrated. As input chief.exe will use the PRECOMMO_UBUF and PRECOM_BLOCKS files generated by preproc, and the RSS9102020000 and RSW9102020000 restart files created by preset. The result should be:

- An ascii output file output/chief.
- Four restart files in WamC5/restarts: RSS9102020100, RSW9102020100, RSS9102020200 and RSW9102020200. The files for 01h00m have been produced for reasons of check-pointing (see Section 5.2).
- A jobs/adtape file, on which the nonlinearities of the forward model were stored.
- A jobs/postmod_020000_020200 ascii file containing results of the adjoint run and the finite difference check.

7.2 Changing the setup

In this subsection it is described how the user can adapt the WAM-ADWAM system to his or her application.

7.2.1 Paths

For large applications it might be desirable to store the sizable restart spectra to scratch. The path of the directory to which restart spectra should stored is defined in the user input files (in jobs/input). For the setup of the test run this was the ../restarts directory. In addition restart files are labelled with a three-character run id. This id is specified in the user input files, and can be very helpful to distinguish between results from different runs (to discriminate between a fine and coarse runs for example).
The paths of the executables are set in the makefiles in the src/prepoc, src/preset and src/chief directories.
The bathymetry and current files are linked to the appropriate Fortran units in the jobs/preproc.job file, which takes care of the execution of the preproc module.

7.2.2 The model dimensions

The maximum allowed model dimensions are defined in the header files located in the src/include directory. The modeldims.h files contains the definitions of maximum allowed dimensions of quantities that are related to the WAM integration part. Amongst others, this contains the maximum number of grid points, frequencies and directions.
The dimensions of the wind input grid are defined in the windpar.h; those of the current field (if used) can be found in the currpar.h file.
In cadj.h the quantities that are relevant for ADWAM are defined. The number of control variables is set here, as well the medium to which the nonlinearities should be written (AMCDEVICE = MEMORY or FILE).

7.2.3 The WAM grid definition

The definition of the numerical grid on which the system will be integrated can be specified in the user input file for the preproc module. This file is located in the jobs/input directory. Here, the following is defined:

- the number of directions and frequencies that are actually used in the model integration.
- the minimum frequency (FR(1)).
- the location and resolution of the spatial grid.
- the location of specified output points.
- if used, the edges of a finer grid.

7.2.4 Timing

The start and end date of the integration as well as the various time steps are set in the user input file chief (in the jobs/input directory):

- The time between two propagation steps (IDELPRO).
- The time between two source integration steps (IDELT).

- The period for which the wind fields at the WAM grid remain unaltered (IDELWO).
- The period between the reading of two external windfields on the wind grid (IDELWI).
- The length of each check-point run (ICHECK).

7.2.5 Model options

The model options are defined in the user input files, located in the jobs/input directory. The most important options are:

- Integration on a spherical (ICASE=1) or a rectangular (ICASE=0) grid.
- A deep water (ISHALLO=1) or a shallow water (ISHALLO=0) run.
- No refraction terms (IREFRA=0), inclusion of depth refraction (IREFRA=1), or inclusion of depth and current refraction (IREFRA=2).
- Only a forward run (IADJNT=0) or both a forward and adjoint run (IADJNT=1).
- Coarse grid run (IBOUNC=1) and/or fine grid run (IBOUNF=1).

7.2.6 The control variables

The connection between the control variables and the WAM model is established in the subroutine XCONNCT, which may be found in the wam.cpp file of the src/chief directory. Here the user may define the control variables to be an initial wave field, model parameters or wind fields. For these choices only the XCONNCT routine needs to be modified. If the user would like to take other quantities as control variables, he or she should make the connection in routines inside the WAM program. However, it is hoped that most choices of control variables can be covered by a modification of XCONNCT only.

7.2.7 The cost function

The connection between the model and the cost is defined in the subroutine NEWCOST, which is located in the wam.cpp file in the directory src/chief. For most applications only this routine needs to be updated. The addition of a penalty for a deviation between an initial guess of some fileds and their actual values, can be made in the routine XCONNCT.

7.2.8 The assimilation scheme

The routine WAVEMDL calculates, based on the values of a set of control variables, a cost. The routine ADWAVEMDL calculates the gradient of the cost with respect to the control variables. Both routines are called in the program CHIEF. In the test case, a finite difference test is made, just to demonstrate that the gradient produced by ADWAVEMDL is correct. For a realistic application, the cost may be optimised, or the gradient may be used for a sensitivity study. The control of how to use WAM and ADWAM can thus be defined CHIEF. For instance, this is the place were a minimising routine (which has to be provided by the user) can be included.

8 Summary

This manual gave a description how to use the WamC5 system, which allows for adjoint runs of the WAM model.
The forward model takes as input a set of control variables. On the basis of their values, the WAM model is integrated. As output a cost is returned which, for instance reflects the agreement between model results and data.
The adjoint model calculates the gradient of the cost with respect to the control variables. As input it sets the adjoint variable corresponding to the cost to one and the remaining ones to zero, as output it returns the adjoint variables of the control variables, which are equivalent to the gradient. The adjoint model was constructed automatically from the WAM source code, by the use of the Adjoint Model Compiler (AMC). The result, ADWAM can be used under the following model options:

- Deep and shallow water,
- Propagation on a spherical or rectangular grid,
- with or without depth and/or current refraction,
- nested grids: only when either the coarse or fine grid is constant, i.e does not depend on the control variables or does not influence the value of the cost function.

It is not applicable for:

- Multi-block runs.

As control variables can be used:

- Model constants,
- Initial wave fields,
- Forcing wind fields,
- Bathymetry dependencies, such as water depths and the local strength of the bottom dissipation. The adjoint for the water depth is not entirely correct, because the dependencies on the dispersion relation have been omitted.

There is no restriction on the choice of the cost function.
To reduce the amount of nonlinearities to be stored, the check-point method has been installed. This can give rise to a large reduction of the required storage, especially when the number of time steps is large. The price one has to pay is that now the forward model has to be run twice to enable an adjoint run, instead of only once.
The adjoint model will calculate the correct local gradients, however, due to the numerical noise in the model, this may be very different from the more global behaviour of the cost function.

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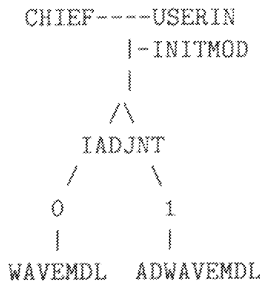

Figure 1: Flow diagram for the supervising routine CHIEF.

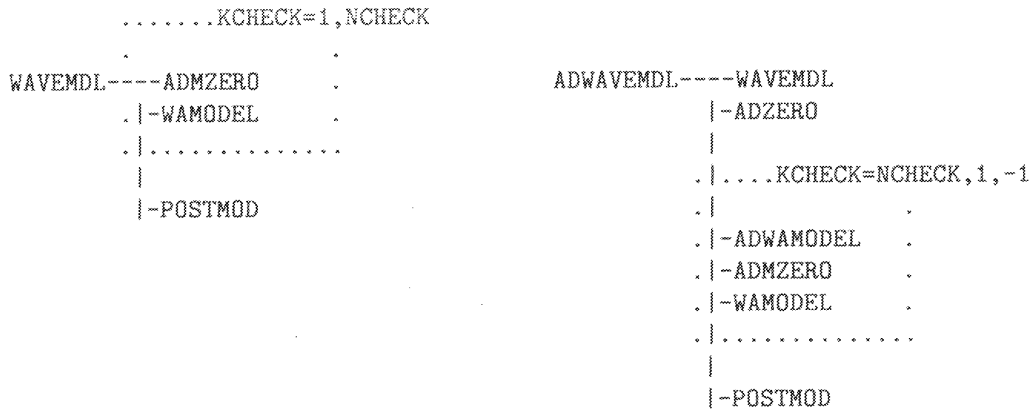

Figure 2: Flow diagrams for the WAVEMDL (left panel) and ADWAVEMDL (right panel) modules. These routines control the check-pointing discussed in Section 5.2.

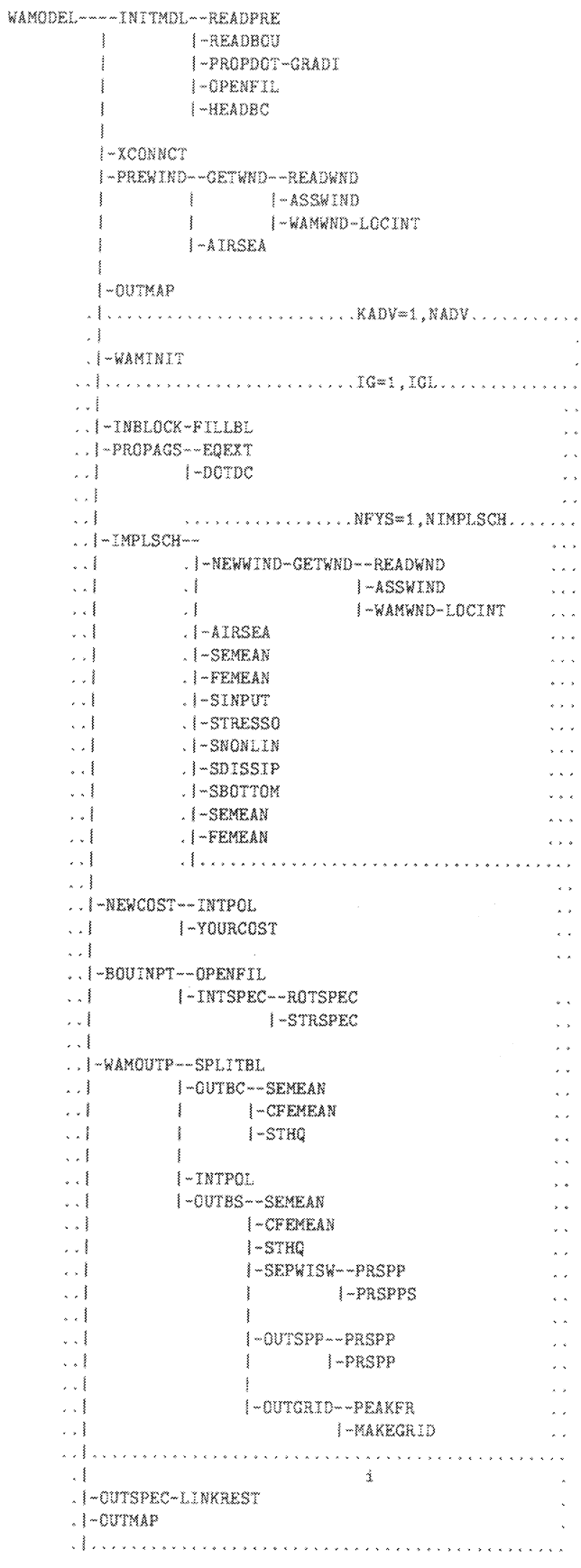

Figure 3: Flow diagram for the WAMODEL module. This routine performs the actual WAM integration.

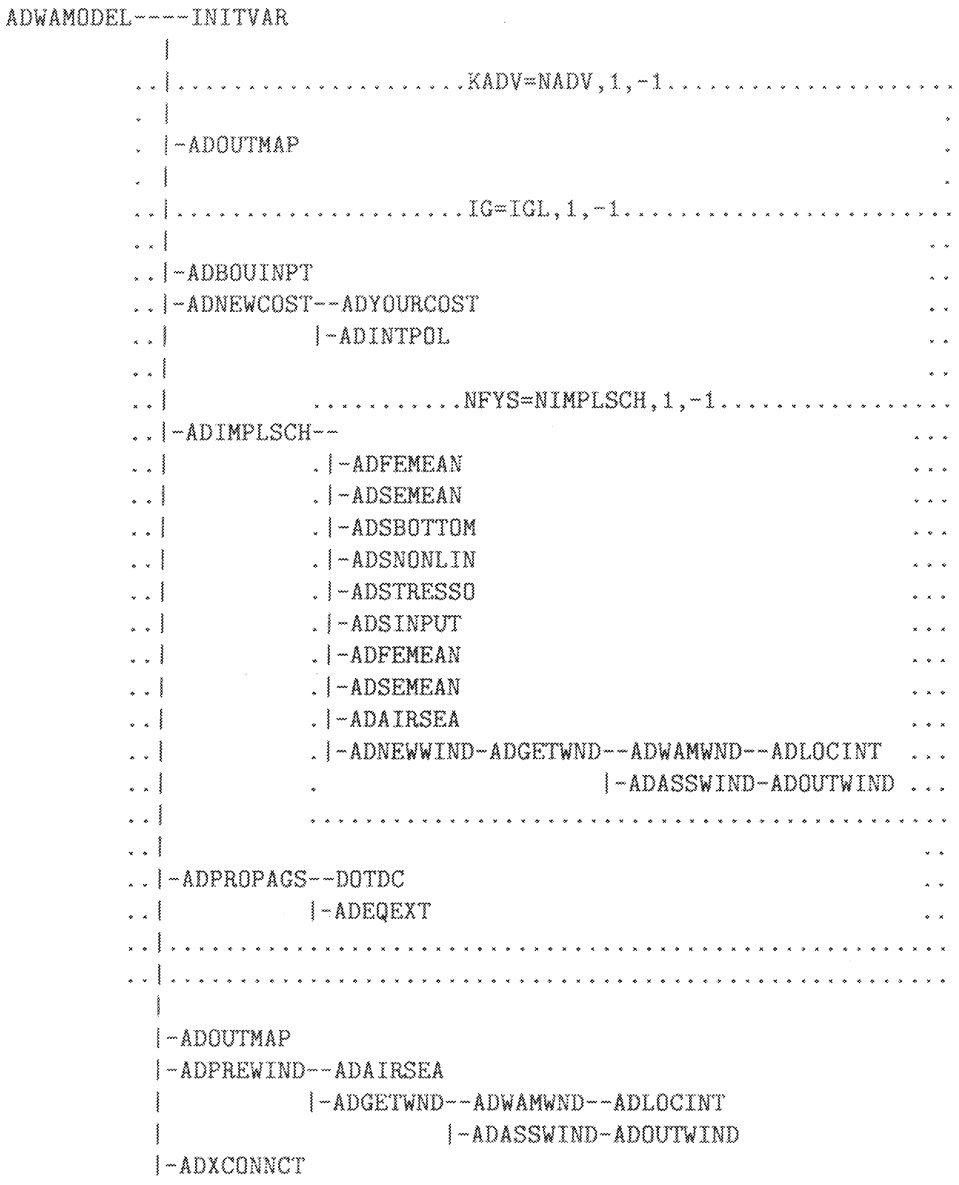

Figure 4: Flow diagram for the ADWAMODEL module. This routine performs the actual adjoint integration of the WAM model. It was generated by AMC.

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