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Development and Testing of Tangent Linear Model for WAVEWATCH III

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14. ABSTRACT
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NRL MEMORANDUM REPORT

Development and Testing of Tangent Linear Model for WAVEWATCH III

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Abstract:

This report describes the construction and initial testing of a linearized, or tangent linear (TL), version of the wave model WAVEWATCH III® (WW3DG 2023; henceforth "WW3"). The TL model is the first component of a variational data assimilation system that is being built for WW3. This system will ultimately also include a complete adjoint model and be integrated into a conjugate gradient error minimization system within NCODA v5. The present document provides details on the selection of subroutines for linearization, the methods by which they were linearized and individually validated, and sample results from individual validations. Preliminary testing of the complete TL model produced some evidence of instability, which we are currently still investigating.

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1 INTRODUCTION

This report documents the creation of a linearized version of WW3. The work described below is part of a three-year 6.2 project, "Developing a Spectral Wave Data Assimilation System for WAVEWATCH III®", funded for FY23-FY25. The project was motivated by a number of performance issues with WW3 and is intended to result in significantly more accurate operational model forecasts, particularly in specific problem areas where wind forcing is the dominant error source.

WW3 Performance Issues

The generally positive results obtained by WW3 in global forecasts sometimes mask more disappointing model performance at the regional and local level. Ship routing officers at the Navy's Fleet Weather Centers (FWCs) continue to encounter and report specific wave environments in which even OI-corrected WW3 forecasts have diverged greatly from the observed wave state. In one such incident, a south Pacific storm system generated a wave spectrum with a second peak in swell heights that was entirely missed by WW3. Wave height errors of several meters are also frequently reported in the Southern Ocean, where a lack of observations and rapidly changing conditions can cause WW3 forecasts to lag behind actual sea states. Comparable model failures are also common in the winter months near large boundary currents like the Kuroshio, when strong opposing winds can produce waves that exceed WW3 forecasted heights by more than 3m.

Advantages of a Variational System for Wave Spectra

Operational global wave models in the U.S., Europe, and Japan – the current state of the art – are generally limited to assimilating only significant wave height (Hs), consequently making a crude bulk correction to total spectrum energy based simply on wave height differences. This approach neglects the specific details of the many waves in any given location that are represented in each frequency directional spectrum, looking only at the total energy integrated over all the different wave types. The data assimilation (DA) system being developed in this project assimilates complete wave spectra, applying a model correction to wind forcing for each wave frequency and direction. In this system, each wave type's energy and direction can individually change, resulting in a corrected model forecast with many waves of new amplitudes traveling in new directions at new speeds. These model corrections will be optimized and true to model physics (in a linearized form).

2 MODEL DESCRIPTION

The wave model used for this project is WAVEWATCH III, version 7.14, which is the latest available version of the model at the present time. To keep the project goals manageable, linearization is limited to just the subroutines that are utilized in operational simulations run by Fleet Numerical Meteorology & Oceanography Command (FNMOC). We have elected to create a DA system for this latest available version of WW3 in the expectation that this version will soon be adopted by FNMOC as its operational version, which would facilitate an easier adoption of the closely matched assimilation system along with it.

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The governing equation of WW3 is the action balance equation, based on the evolution of the action density, N (i.e., energy density, E, normalized by angular frequency, σ). In simplified form, it may be expressed as:

$$\frac{\partial N}{\partial t}+\frac{\partial C_x N}{\partial x}+\frac{\partial C_y N}{\partial y}+\frac{\partial C_\sigma N}{\partial \sigma}+\frac{\partial C_\theta N}{\partial \theta}=\frac{S}{\sigma} \tag{1}$$

The action density is a function of location, frequency, direction, and time: $N = N(x, y, \sigma, \theta, t)$. Relative wave frequency σ is measured from a frame of reference moving with any existing current, and θ is wave direction. C is the wave action propagation speed in both geographic and spectral space, with subscripts indicating the component of group velocity (C_g) in the x, y, σ, and θ axis directions. The right-hand side of (1) is the sum of all source/sink terms normalized by frequency, $S = S(x, y, \theta, \sigma, t)$. In v7.14 and other recent versions of WW3, this sum includes components $S_{in} + S_{nl} + S_{ds} + S_{bt} + S_{ice}$; i.e., input by wind, nonlinear interactions, dissipation, bottom drag, and wave-ice interactions, respectively. For each propagation component and source/sink term, the model offers multiple computation options that may be selected by the user. Only the subroutines associated with user-specified computation options are included in the compiled WW3 executable.

3 BUILDING AND TESTING THE TANGENT LINEAR MODEL

Linearization of a large computer model such as WW3 can be laborious and time-consuming, as it requires that each line of the code be inspected and linearized if/when necessary. For this project, we purposely chose to limit the linearization to only the model components that are utilized in the Navy's operational version of the code by FNMOC. This decision significantly reduces the list of subroutines to be processed and facilitates the completion of this project within its proposed three-year timeframe. Several methods were employed to create the linearized components of WW3, including purely manual code writing, utilization of automatic differentiation software packages, or some combination of these two.

The subroutines that are used by FNMOC in the operational version of WW3 are presented in a simplified model architecture chart in Figure 1. Color coding in the figure indicates which routines require processing for this DA system and which stages of that processing have been completed as of the date of this report. Tangent linear subroutines have been created and validated for all primary components of the operational model; the highest-level routines shown in the figure (**ww3_multi** and **wmwave**) are primarily wrapper routines designed to manage the overall computation, sharing information about multiple grids among multiple compute nodes. They require only limited modifications to accommodate the lower-level TL and adjoint components of the model.

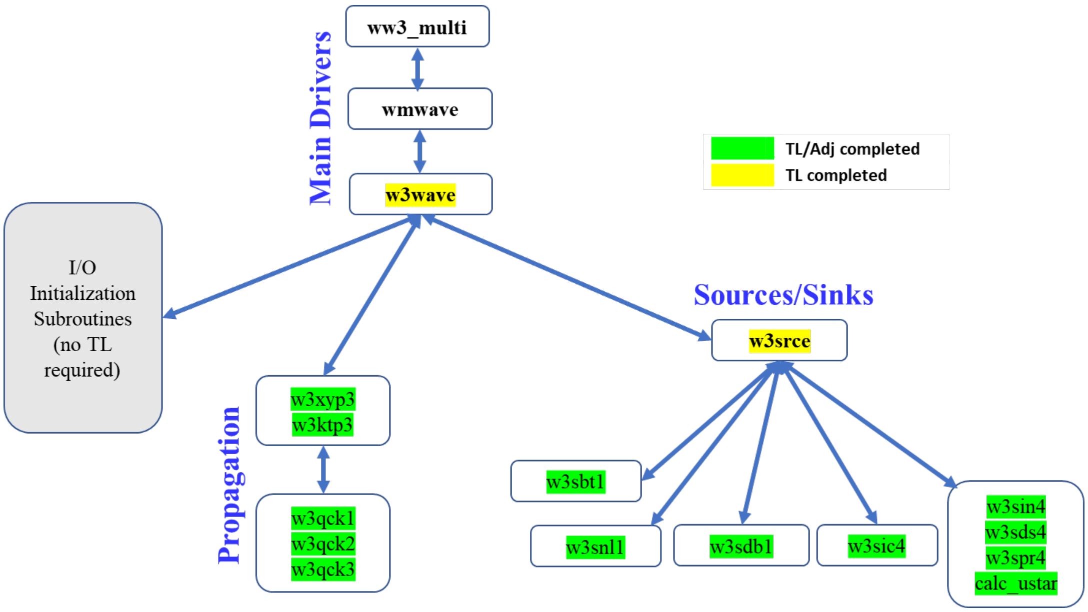

Figure 1. Processed subroutines from operational WW3 model.

3.1 Construction of Individual Tangent Linear Subroutines

As noted above, the linearization of a Fortran-based computer model generally requires an examination and linearization of each of the lines of code in the relevant parts of the model. Nonlinear expressions such as those that compute the square, cube, or square root of an active variable must be replaced with linear approximations of those expressions. For example, in the following nonlinear Fortran expression from WW3,

$$CD = (USTAR/UNZ)**2 \qquad (2)$$

all three variables (CD, USTAR, and UNZ) are dependent on the primary active variable (i.e., wave action A), so that each of them must be included in the linearization. Consequently, the linearized (TL) form of (2) would be written as follows:

$$CD\_TL = (2.0*USTAR/UNZ)*((USTAR\_TL/UNZ)-(USTAR*UNZ\_TL/(UNZ**2.))) \qquad (3)$$

where the appended expression "_TL" designates a given variable as the (small) perturbation of the original variable.[2] In this case, the tangent linear version of WAVEWATCH III would produce a linearized estimate of the nonlinear variable CD that would be computed as

$$CD\_est = CD\_0 + CD\_TL \qquad (4)$$

In (4), the updated value of CD (CD_est) is calculated by adding the perturbation CD_TL to a previously computed "background" (unperturbed) value of CD (CD_0).

[2] To promote stability, some linearized expressions like (3) were rewritten in simpler form in the TL model by replacing selected dependent variables with their background values.

A majority of the TL subroutines that we created were constructed manually (primarily by co-authors HN and MC), occasionally with assistance from the Parametric Fortran Compiler (PFC) auto-differentiation tool (Erwig et al., 2007). A somewhat smaller number were generated (by co-authors MO and JV) using the automatic differentiation software Tapenade (Hascoet & Pascual, 2012; https://team.inria.fr/ecuador/en/tapenade/). The PFC utility is described in more detail in Orzech et al. (2013). Our work with Tapenade is described in greater detail in the next section.

Tapenade Auto-Differentiation Utility

Tapenade is available in the public domain and can often be a convenient way to efficiently create TL and adjoint subroutines. The differentiator may be employed either at the command line of a linux-based operating system or online using the web interface for the Tapenade server (accessible at http://www-tapenade.inria.fr:8080/tapenade/index.jsp). For the auto-generation of selected TL routines (and a majority of required adjoints), we primarily utilized the command-line version of Tapenade. For less complex routines, the tool proved generally very effective and efficient, producing a new TL or adjoint for a specified subroutine within just seconds of entering the primary command. However, for more complex routines, Tapenade sometimes had difficulty creating consistent TLs and/or adjoints, particularly if the original routines included highly nonlinear expressions involving many dependent variables, multi-nested max/min statements, and/or multi-condition if/else statements. In such cases, we reverted to the manual construction method.

For the cases where we did employ Tapenade, we also identified a few other minor configuration peculiarities that required additional pre- and/or post-processing. The differentiator did not recognize specially marked "#ifdef" code lines that are included in the WW3 v7.14 to indicate portions that should be removed by the C-based preprocessor, so these lines had to be commented out or removed before calling Tapenade. After the TL routine was created, we also needed to perform minor additional cleanup work such as removing INTRINSIC declaration statements inserted into the TL for basic functions (i.e, SQRT or SIN) and replacing Tapenade's appended letter "b" to designate each TL variable with our own preferred "_TL". Co-authors JV and MO developed separate python scripts to automatically perform most of this pre- and post-processing (available to other modelers upon request).

Once the minor corrections were completed, little or nothing else was generally required to produce a fully valid TL subroutine. Each new subroutine was then individually validated with the perturbation tests detailed in Section 3.2 below.

3.2 Validation of Individual Subroutines

Each TL subroutine was validated by applying two different standardized perturbation tests to the active and dependent variables in each function, with the model compiled and run in double precision. In both types of test, the output of the TL model is compared to the difference of perturbed and unperturbed outputs of the original nonlinear model. In a series of repeated simulations, the perturbation of each input variable is iteratively set to a decreasing fraction of the original value of the variable. In symbolic form, the vector of output variables $\vec{Y}$, generated by applying the original nonlinear subroutine F to input vector $\vec{x}$, may be written as

$$\vec{Y} = F(\vec{x}) \tag{5}$$

and the vector output of the perturbed nonlinear model and of the tangent linear model are written, respectively, as

$$\begin{aligned} \vec{Y}_P &= F(\vec{x} + \varepsilon\vec{x}) \\ \vec{Y}_{TL} &= F'(\vec{x})\varepsilon\vec{x} \end{aligned} \tag{6}$$

where F' is the differential or linearized version of F and ε is the perturbation factor (set initially to 0.1 for all of our validations). At each step of the iteration, both a TL and a perturbed output are computed based on a decreasing value of perturbation $\varepsilon = (\varepsilon_0)^n$. In these tests, we have set $\varepsilon_0 = 0.1$ and n = 1 to 9. For each active output variable Y_i and perturbation factor ε, the values of TL outputs, $\vec{Y}_{TL}$, are compared to the differences in outputs generated by the original nonlinear subroutine with perturbed and unperturbed inputs (i.e., $\vec{Y}_P - \vec{Y}$). A slightly idealized model domain was created for these tests (Figure 2), featuring multiple irregular coastlines, shallow regions, and an artificial iceberg.

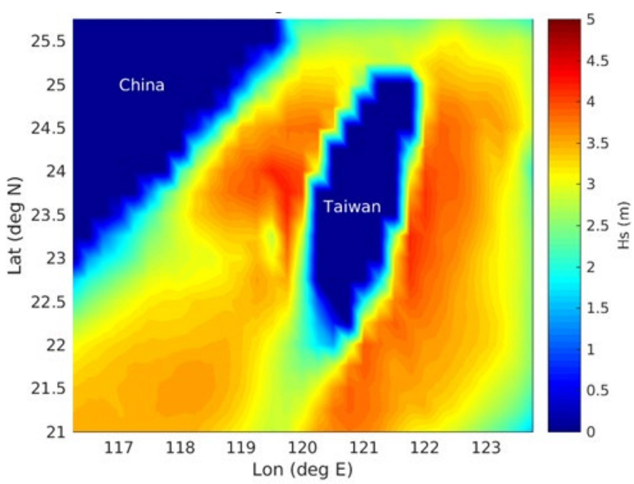

Figure 2. Model test domain (South China Sea region), including model-estimated significant wave height values for a single timestep in January 2021. To facilitate testing of model's wave-ice interaction component, an idealized "iceberg" was inserted into the domain at approximately 118°E, 23°N.

Validation Method #1: Ratio Test

For the first validation method utilized in this analysis, the test is based on a *ratio* of the sums of magnitudes of these two vectors:

$$\delta = \frac{\sum_i \left|Y_{P,i} - Y_i\right|}{\sum_i \left|Y_{TL,i}\right|} \tag{7}$$

In (7), the values in the numerator and denominator are summed over all components of the output vectors, which generally include multiple output variables, geographic locations, and spectral bins. Ratio values are expected to be close to 1.0 (i.e., $|1.00 - \delta| < 10^{-1}$), except in cases where the output of the original subroutine is only a linear function of the input (which causes $|1.00 - \delta|$ to be zero, to machine precision, for all values of ε). In a successful validation, we expect to find that the value of |1 – δ| initially decreases as the perturbation factor ε is reduced, ultimately reaching values of order 10^{-8} before finally increasing again for the very smallest values of ε (due to limits of machine precision). An example of the results from a successful test of the TL of subroutine W3SIN4 is provided in Table 1 below. The ratio test was used to validate all TL subroutines other than the "Main Drivers" shown in Figure 1 (which were validated using the method described in Section 3.3 below).

Table 1. Example of TL Validation Test Output – Eqn (7) formulation (W3SIN4_TL)

ii	**ε**	**δ**	**|1 – δ|**
1	1.0e-01	1.001237795152119	1.24e-03
2	1.0e-02	1.000142262907607	1.42e-04
3	1.0e-03	1.000014464657321	1.45e-05
4	1.0e-04	1.000001448934150	1.45e-06
5	1.0e-05	1.000000144938380	1.45e-07
6	1.0e-06	1.000000014208187	1.42e-08
7	1.0e-07	1.000000018539392	1.85e-08
8	1.0e-08	0.999999996883369	3.12e-09
9	1.0e-09	1.000002956539849	2.96e-06

Validation Method #2: Difference Test

For the second validation method utilized in this analysis, the *difference* of the three types of model outputs is computed instead of the ratio, i.e.:

$$\Delta = \sum_i \left| (Y_{P,i} - Y_i) - Y_{TL,i} \right| \tag{8}$$

In this case, when the original routine is fully nonlinear and the TL subroutine is correctly formulated, the value of Δ in (8) will decrease with decreasing ε at a rate proportional to ε^2. This validation method is considered more robust than that described in (7), because it more consistently detects cases where the TL code has been erroneously multiplied by a unitary (or "nearly unitary") matrix. In such cases, the value of |1 – δ| based on the ratio in (7) can sometimes still attain values of order 10^{-8} as ε decreases (suggesting a valid TL subroutine), but the difference in (8) will always decrease more slowly than ε^2 (correctly indicating an error in the TL code).

An example of the results from a successful test of the subroutine W3SIN4_TL using the second validation method is provided in Table 2.

Table 2. Example of TL Validation Test Output – Eqn (8) formulation (W3SIN4_TL)

ii	ε	Δ	Δ/Δ_1
1	1.0e-01	1.06e-01	1.00
2	1.0e-02	9.25e-04	9.80E-03
3	1.0e-03	9.17e-06	9.72E-05
4	1.0e-04	9.17e-08	9.72E-07
5	1.0e-05	9.17e-10	9.72E-09
6	1.0e-06	9.17e-12	9.72E-11
7	1.0e-07	9.08e-14	9.62E-13
8	1.0e-08	5.19e-16	5.50E-14
9	1.0e-09	4.85e-16	5.14E-14

In the final two rows of the table, the value of Δ has become small enough that it reaches the limit of machine precision. As a consequence, its value does not continue to decrease as ε^2 for the final two values of ε.

The difference test was successfully applied to all individual TL subroutines in the "Propagation" and "Source/Sink" groups of Figure 1 except **w3srce**, for which the value of Δ/Δ_1 only decreased as ε^1 (Note that this subroutine *was* still successfully validated using the ratio test above)[3]. Detailed results for all difference tests of individual subroutines based on Eqn (8) are provided in the Appendix (Section 6) with additional commentary where appropriate.

3.3 Evaluation of Complete TL Model

Preliminary evaluation of the complete tangent linear model is accomplished by applying a similar, somewhat more cumulative comparison test to the model's final output variable, the wave action spectrum, after perturbing the model's primary input variable, the wind forcing. In this test, the TL model output of tangent linear spectra is compared to the difference of spectral outputs from two runs of the nonlinear WW3: (***a***) WW3 with unperturbed original wind forcing, and (***b***) WW3 with perturbed wind forcing. The wind forcing input to the TL model run is the same as the perturbation applied to wind forcing in run ***b*** of the nonlinear model. If the tangent linear model is functioning properly, it will produce a result in which the spectral output increases linearly with the perturbation for all perturbation sizes. In contrast, the perturbed nonlinear model will diverge quadratically from the unperturbed nonlinear model as the perturbation size is increased.

We conducted three sets of simulations to compare these different outputs, featuring model runs of 30 minutes, 6 hours, and 12 hours in length. At the beginning of each set, the unperturbed nonlinear WW3 model was run once for the model domain, and its spectral output was saved. Then, for each run of the test series, the perturbation factor was applied to the magnitude of the wind forcing throughout the domain and used both to initialize the TL model and to perturb an initialization of the nonlinear model. For each test set, perturbations were computed as a percentage of the original wind magnitudes, ranging in size from 0.1% to 10%. Model output in

[3] The output of subroutine w3srce is based on output parameters generated by the eight individual source/sink routines that it calls. Some of these parameters are computed as linear functions of associated input variables, and their inclusion in the computed output of w3srce acts to disrupt the results of the difference test, which is only designed for testing nonlinear output variables. See appendix for more examples of this linear output effect.

each simulation was quantified by summing the magnitudes of all bins of the wave action spectra (or TL spectra) over all domain locations upon completion of each run.

Comparison of outputs |P-U| and |TL|

The sum of absolute differences of perturbed-minus-unperturbed WW3 output ("P-U") is plotted versus perturbation size together with the sum of absolute TL WW3 output for the 30-min, 6-hr, and 12-hr model runs in Figure 3 – Figure 5.[4] In each figure, the nonlinear |P-U| output increasingly diverges from the linear |TL| output with growing perturbation size, and this divergence becomes larger with increasing simulation time. For each set of simulations, the differences between |P-U| and |TL| output are generally small (less than 1% of the total TL output) for perturbations under one percent, but they grow rapidly (to over 20%) for wind forcing perturbations of five percent or greater. The divergence rates of these outputs with increasing time and perturbation size will ultimately play a role in determining the size of the assimilation window in time and space for the completed data assimilation system.

Somewhat surprisingly, the results from the 12-hr simulations (Figure 5) appear almost identical to those from the 6-hr simulations (Figure 4), while the total wave action levels in these two plots are all considerably larger than those from the 30-min simulations. Intuitively, it would be expected that the system error would continue to grow over time as the additional wind forcing continued to increase wave energy levels in the perturbed model versus the unperturbed model. In the present simulations, however, this effect may have been dampened somewhat, because the wind forcing and wave energy in the test case were decreasing in the model domain during this 12-hr time period. Total wave action in the unperturbed simulation was computed to be 3.25×10^4 after 30 minutes, but only 2.75×10^4 after 6 hours and 1.8×10^4 after 12 hours.

[4] |P-U| values are determined by first computing the difference for every frequency and directional bin at every location, then taking the absolute value of the differences, and then summing the result. Values of |TL| are computed by taking absolute value of all datapoints, then summing.

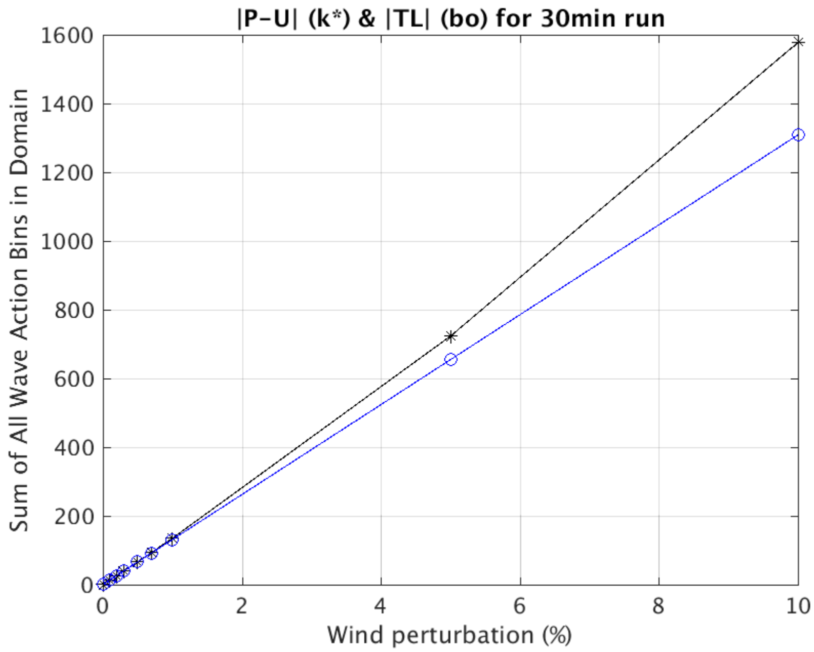

Figure 3. Comparison of total energy density output (TL WW3 and perturbed-minus-unperturbed WW3) plotted versus wind forcing perturbation size. Model run time was **30 minutes**.

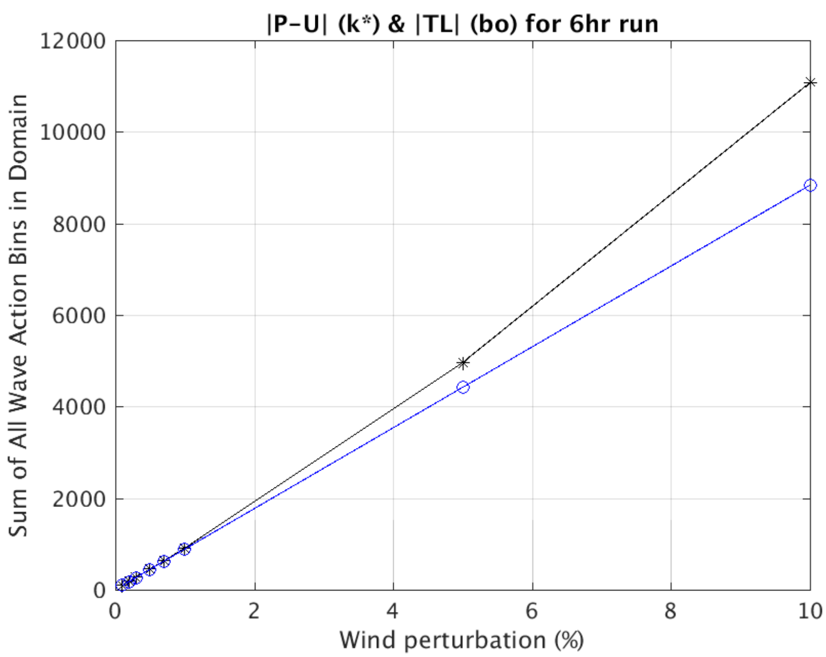

Figure 4. Comparison of total energy density output (TL WW3 and perturbed-minus-unperturbed WW3) plotted versus wind forcing perturbation size. Model run time was **6 hours**.

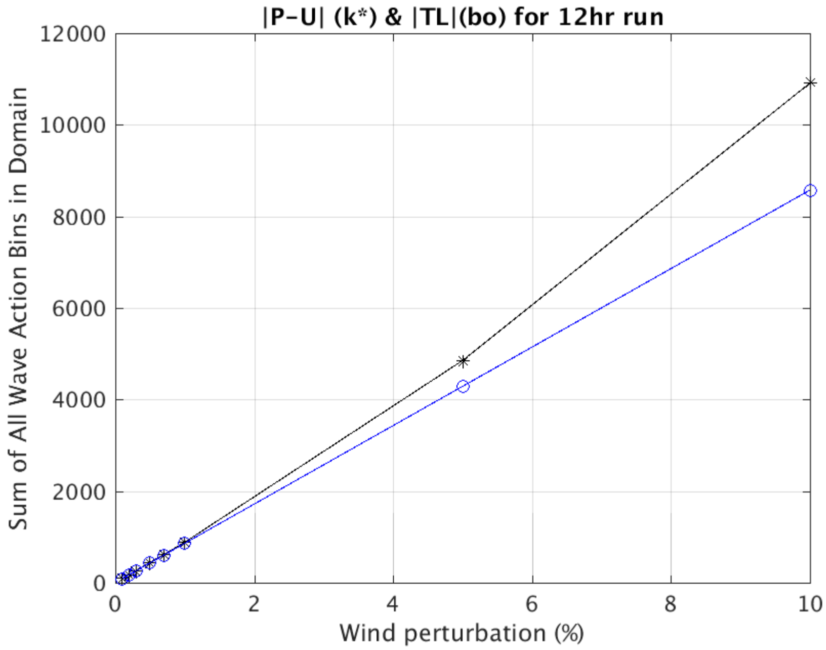

Figure 5. Comparison of total energy density output (TL WW3 and perturbed-minus-unperturbed WW3) plotted versus wind forcing perturbation size. Model run time was **12 hours**.

Difference of all outputs |P-U-TL|

To confirm the convergence of the perturbed-minus-unperturbed and the TL results at the smallest scales, we now examine the absolute difference of all outputs (i.e., |P-U-TL|) for very small perturbations for all three model run times (Figure 6 – Figure 8). The best-fit quadratic polynomial for each dataset is also plotted in each figure, and the RMS error for each curve is provided in the caption along with its quadratic equation.

All three figures show a clear nonlinear trend in the absolute difference data with increasing perturbation size, indicating that the TL model is correctly formulated and does not include significant erroneous nonlinear components. Upon visual comparison, the 6-hr and 12-hr difference values appear to fit the quadratic curve better than the 30-min values. On an absolute basis, however, the RMS error values for the data points relative to the curve are of the same order for all three sets of tests (RMSE=0.25 for the 30-min data, 0.21 for the 6-hr data, and 0.11 for the 12-hr data). Relative to the total wave action in the domain for each test, the summed |P-U-TL| difference value for a one percent wind perturbation is still very small, constituting 0.025%, 0.18%, and 0.33% of total action in the 30-min, 6-hr, and 12-hr test cases, respectively.

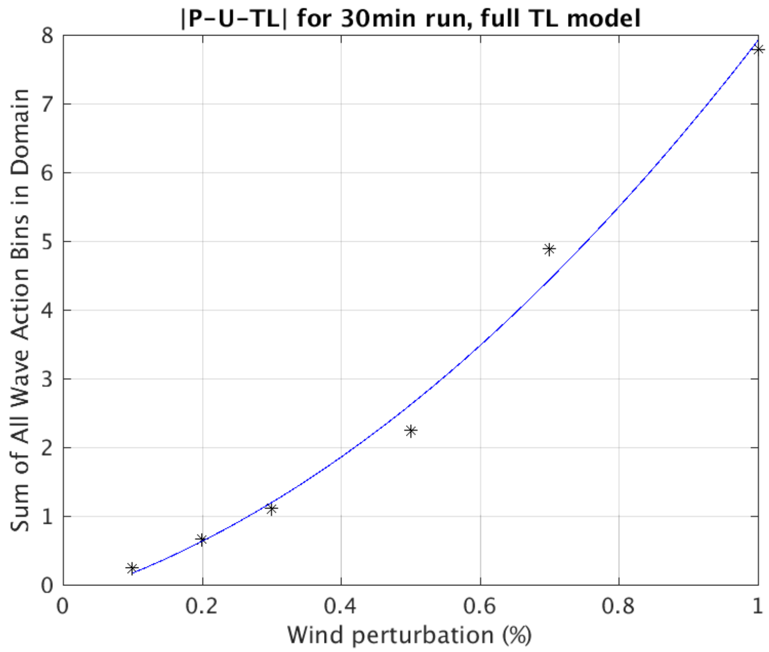

Figure 6. Absolute difference of total wave action (perturbed-minus-unperturbed minus TL), plotted versus wind forcing perturbation size after **30-min** simulation, smaller perturbations only. Best-fit curve (blue line) follows polynomial $y = 4.98x^2 + 3.14x - 0.2$. RMS error of data points is 0.25. Normalized by the curve value at 1% wind perturbation, this is 0.032.

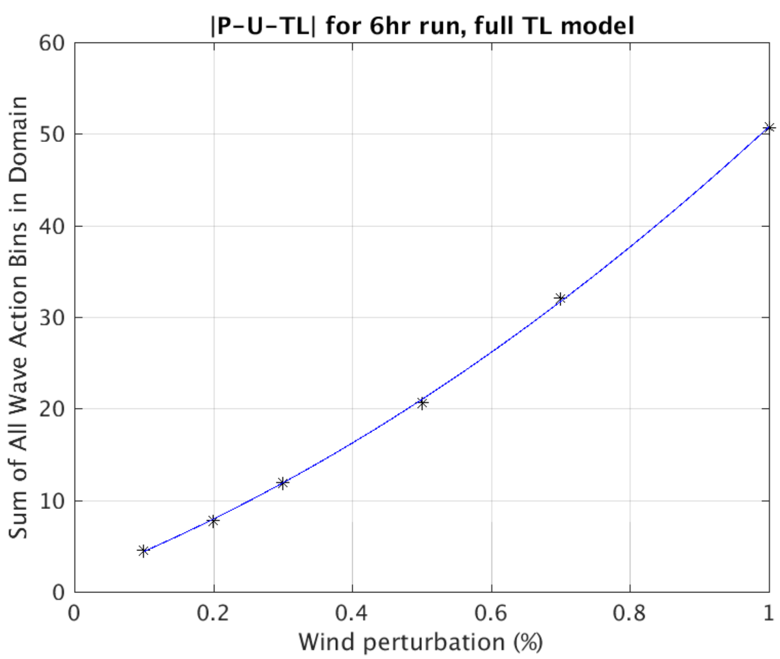

Figure 7. Absolute difference of total wave action (perturbed-minus-unperturbed minus TL), plotted versus wind forcing perturbation size after **6-hr** simulation, smaller perturbations only. Best-fit curve (blue line) follows polynomial $y = 20.13x^2 - 29.4x + 1.23$. RMS error of data points is 0.22. Normalized by the curve value at 1% wind perturbation, this is 0.004.

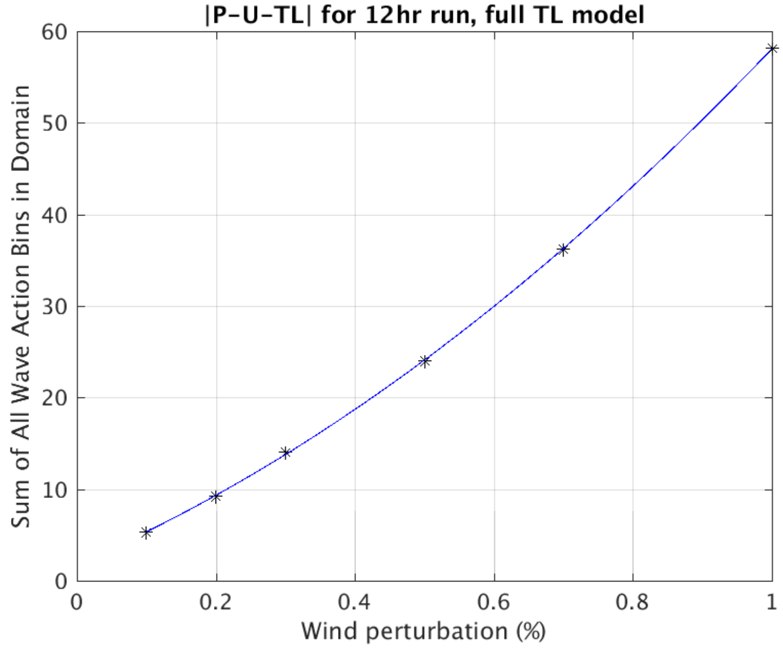

Figure 8. Absolute difference of total wave action (perturbed-minus-unperturbed minus TL), plotted versus wind forcing perturbation size after **12-hr** simulation, smaller perturbations only. Best-fit curve (blue line) follows polynomial $y = 23.46x^2 + 32.8x + 1.81$. RMS error of data points is 0.11. Normalized by the curve value at 1% wind perturbation, this is 0.002.

Total of all TL outputs versus time

To examine the TL model's behavior and stability over time, the total wave action output of the TL model is saved at regular intervals over a 1-day period, using wind forcing perturbation levels ranging from 0.1% to 10% in five different simulations. The combined results from all the simulations are provided in Figure 9.

For a correctly functioning tangent linear model, it is expected that the TL output will initially change linearly over time, indicating a stable computation. Depending on the specific characteristics of the model, this steady linear evolution will eventually shift to a much more rapid nonlinear growth, indicating model instability. In the case of the TL model for WW3, we find that the system remains stable for between 10 – 15 hours, depending on the perturbation size.

This result suggests that, when this TL model is incorporated into the complete WW3 data assimilation system, it may be possible to use an assimilation period of up to 12 hours for corrections to the nonlinear model if perturbations remain small. If wind innovation/error values produced by the adjoint model are of order 1% or larger relative to background values, the system would be limited to an even shorter assimilation period, which would not be compatible with requirements of operational forecasts.

Additional tests are still being conducted to fully delineate operational stability limits of the TL model and identify/fix specific sources of instability. They will be described in a future report.

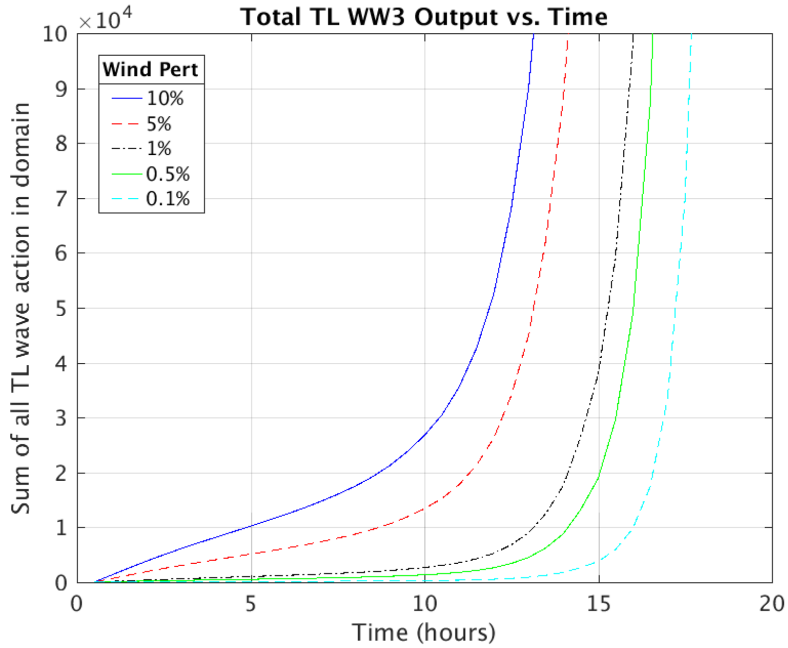

Figure 9. Sum of all TL wave action in model domain plotted versus time for five separate simulations, each of which used a different wind perturbation.

3.4 WW3 Configuration Issues

Lookup Table Effect on Small Perturbation Results

During the tests of the full TL model, we came across two aspects of the WW3 model configuration that affected its output and our results. The first of these is the model's use of a lookup table for quantifying the effects of the wind on the wave spectrum. The wind speed values indexing the lookup table are discrete, and the effects on the wave spectrum are determined by selecting the nearest index value in the table to the actual input wind speed (rather than by interpolating these effects between neighboring table index values). Consequently, if the wind speed difference (or perturbation) is very small (i.e., ≤ 0.1%), the model's estimated spectral modification due to wind can occasionally be exactly the same even when two different wind speeds are used.

This result is illustrated in Figure 10, which shows a zoomed-in view of the "P-U" result from Figure 3, with results computed for a number of additional very small perturbations. As can be seen for perturbation values between 0 – 0.3%, the perturbed-minus-unperturbed WW3 output summed over the domain remains constant for perturbations differing by up to 0.1%, even though the perturbed wind was (slightly) larger than the unperturbed wind. Although it may apply to some special cases, this model limitation is unlikely to have a significant effect on regular model runs, for which wind forcing corrections or errors are usually not all the same small size and are not uniformly distributed.

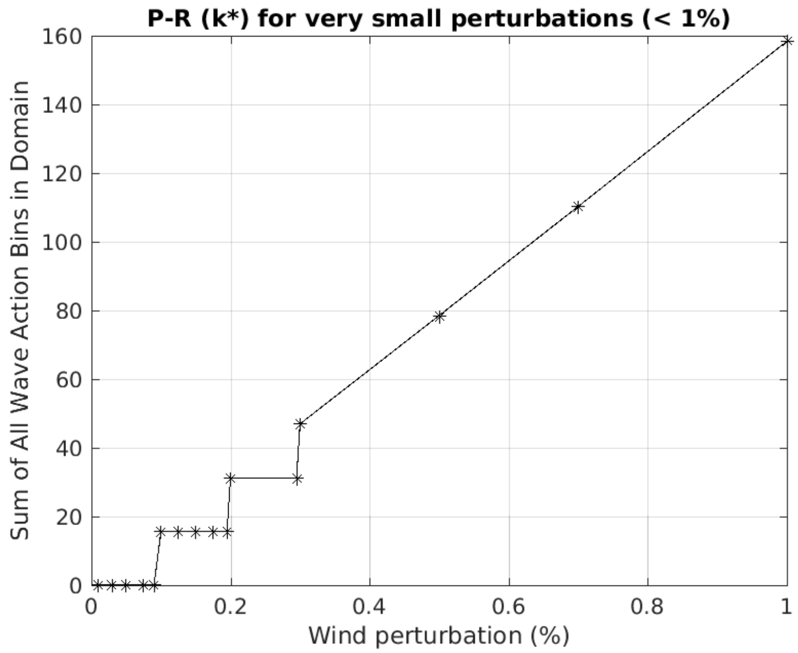

Figure 10. Total energy density output (perturbed-minus-unperturbed WW3) plotted versus wind forcing perturbation size for very small perturbations.

Requirement for Restart File

The second model characteristic that affected our results was a feature of the model setup rather than a bug. We identified the issue when examining results from an earlier 30-minute test case that has since been discarded. The case was initialized with parameterized "warm start" conditions, so that the initial wave conditions throughout the domain, although nonzero, were not entirely realistic. In this case, the wave energy throughout the domain was not distributed in a manner that was fully consistent with the wind forcing, requiring several hours to attain such a state. In the test, this incorrect distribution of wave energy caused the (perturbed-minus-unperturbed) WW3 output to follow a roughly linear trend (Figure 11) instead of the expected nonlinear divergence from the TL curve that would be expected for increasing perturbation size (compare Figure 3 & Figure 11). We were able to resolve the problem by modifying our test configuration to initialize the wave state with a full "restart" (or hotstart) file based on realistic wave conditions from a spin-up run of the model completed for several days preceding the start of our test period.

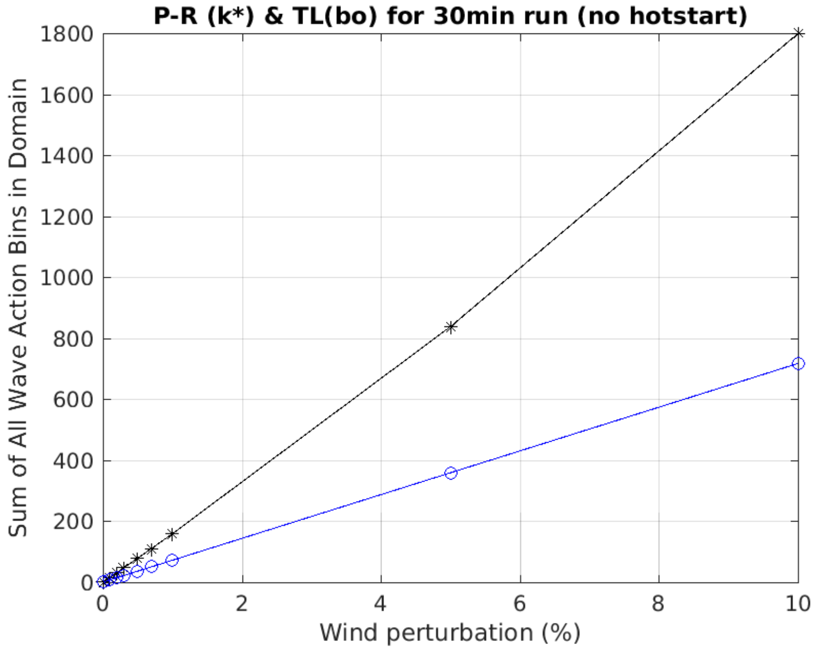

Figure 11. Comparison of total energy density output (TL WW3 and perturbed-minus-unperturbed WW3) plotted versus wind forcing perturbation size. Unlike Figure 2, *these simulations did NOT use a restart (hotstart) file to begin from an authentic ocean state*., which led to a nearly uniform P-U trend for all perturbation sizes (compare to Figure 3). Model run time was 30 minutes.

4 DISCUSSION AND CONCLUSIONS

This report has detailed the consistency testing of tangent linear subroutines created for the components of WAVEWATCH III that are used in the operational model. Subroutines have been tested individually as well as collectively.

Individual subroutines were each tested with both a “ratio test” (as described by Equation (7)) and an “absolute difference” test (as described by Equation (8)). Each test demonstrates the convergence of the TL result to the original nonlinear result for decreasing perturbation size. These tests are designed to work properly only for subroutine parameters that are computed in a nonlinear fashion in the original subroutine. If an output parameter is computed linearly from an active input parameter, or if an output parameter is computed from other values that are not active input variables, these tests will indicate that the subroutine has “failed”. To obtain a successful test result, these types of output parameters should be excluded from the TL tests of individual subroutines. Only output variables that are nonlinear functions of active input variables should be included.

Preliminary collective testing of all TL subroutines was accomplished using essentially a larger version of the “absolute difference” test that was applied to individual routines. In multiple simulations, the model’s wind forcing input was perturbed over a range of perturbation sizes. The complete TL model was then initialized with only the perturbation values for the same range of perturbation sizes. In addition, the difference of total wave spectral outputs from the perturbed and unperturbed original model was compared to the corresponding TL spectral output of the TL model to demonstrate the convergence of these outputs with decreasing perturbation size (Figure 6 – Figure 8). Finally, the total spectral output of the TL model over time was compared for five different initial perturbations, illustrating the initial linear behavior of the TL model followed by the onset of nonlinear instability after a period ranging from 10 – 20 hours.

These combined results suggest that the TL model is configured and generally runs stably for periods of 12 hours or less, with wind perturbations less than 1% of actual wind magnitudes. In an effort to maintain model stability for longer periods (i.e., at least several days), we are now conducting additional tests with a simplified model configuration. We have tentatively replaced the operational switches for source terms (ST4) and propagation (PR3) with the most basic options for these model components (ST1 and PR1, respectively), and we have simplified additional selected lines of code to reduce instability (as described in the footnote to Section 3.1). Results of this effort will be described in a future report.

4.1 Upcoming Work – Adjoint and DA System

As was illustrated in Figure 1, we have completed almost every adjoint subroutine corresponding to each of the TL subroutines described in this report. Each adjoint routine must be validated together with its TL. For this validation, we are using the standard “inner product” test, which is normally expressed as an identity similar to the following:

$$\langle \mathbf{Au}, \mathbf{v} \rangle \equiv \langle \mathbf{u}, \mathbf{A}^{\mathbf{T}}\mathbf{v} \rangle \tag{9}$$

Where $\mathbf{A}$ is a matrix representing the linear actions of the TL model, $\mathbf{A}^{\mathbf{T}}$ is its transpose and represents the linear actions of the adjoint, and the vectors **u** and **v** are the inputs and outputs of these two models. To fully validate the adjoint, the identity given by (9) must be satisfied by each TL/adjoint pair and by the full TL/adjoint models to within machine precision. We have already completed this validation for most individual subroutines, but not yet for the full model.

Following validation of the adjoint model, the TL and adjoint will be integrated into the NCODA data assimilation system as modules, together with a set of estimates of the wind error covariance. The resulting WAVEWATCH III Data Assimilation System will be tested in both regional and global domains with extensive wave spectral datasets from surface buoys (e.g., Sofar; https://www.sofarocean.com) and high-resolution satellites (e.g., CFOSAT; https://www.eoportal.org/satellite-missions/cfosat).

4.2 Dissemination of Code

While the WAVEWATCH III Data Assimilation System is under development at NRL, this code will not be shared with other research organizations. After the system has been fully validated (possibly by FY28), it will be transitioned to operational use by the Fleet Numerical Meteorology & Oceanography Command (FNMOC). A public release date for this data assimilation software is not yet known.

5 REFERENCES

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Hascoet, L., and Pascual, V., 2012: The Tapenade Automatic Differentiation tool: principles, model, and specification. *Res. Rept. #7959*, Inria Project-Team Tropics, 50pp. https://www-sop.inria.fr/tropics/papers/TapenadeRef12.pdf.

Orzech, M., J. Veeramony, and H. Ngodock (2013). "A variational assimilation system for nearshore wave modeling," *J. Atm. & Oceanic Tech*., 30, pp. 953-970, doi: 10.1175/JTECH-D-12-00097.1.

WAVEWATCH III® Development Group (WW3DG), 2019: User manual and system documentation of WAVEWATCH III® version 6.07. *Tech. Note 333*, NOAA/NWS/NCEP/MMAB, College Park, MD, USA, 465 pp. + Appendices. (*Note: This citation refers to an earlier version of WW3, as requested by WW3DG, because version 7.14 is not yet generally available*.)

6 APPENDIX – Detailed Results of TL Tests

The tables included in this section provide explicit results of the testing of each tangent linear subroutine in TL WW3 (tests performed by K. Patel). All these tests are based on values of Δ computed using the "absolute difference" expression of Equation (8). Tests of the two highest level TL subroutines (W3WAVE_TL and W3SRCE_TL) were generally successful

6.1 Tests Completed without Any Issues or Caveats

ii	ε	Δ/Δ_1						
		W3QCK1	W3QCK2	W3QCK3-X	W3QCK3-Y	W3XYP3	W3KTP3	W3SNL1
1	1.00E-01	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
2	1.00E-02	1.15E-01	1.57E-05	3.51E-02	5.96E-02	2.64E-02	3.16E-02	7.89E-03
3	1.00E-03	1.80E-02	4.70E-13	5.06E-09	5.45E-10	1.16E-03	1.86E-04	7.87E-05
4	1.00E-04	7.48E-13	4.70E-13	4.05E-12	5.45E-12	2.10E-13	4.62E-14	7.87E-07
5	1.00E-05	6.53E-13	4.83E-13	9.77E-14	1.30E-13	2.40E-13	4.71E-14	7.87E-09
6	1.00E-06	8.58E-13	5.82E-13	8.49E-14	1.06E-13	2.11E-13	5.13E-14	7.87E-11
7	1.00E-07	8.52E-13	4.98E-13	9.02E-14	1.10E-13	2.39E-13	5.60E-14	7.83E-13
8	1.00E-08	8.35E-13	4.99E-13	8.89E-14	1.11E-13	2.21E-13	5.42E-14	6.42E-15
9	1.00E-09	7.86E-13	4.88E-13	7.84E-14	9.87E-14	2.34E-13	5.14E-14	3.29E-14

W3SIN4 (results obtained for each output parameter)

ii	ε	Δ/Δ_1						
		ALL	VSIN	VDIN	TAUWX	TAUWY	TAUWAX	TAUWAY
1	1.00E-01	1.00	1.00	1.00	1.00	1.00	1.00	1.00
2	1.00E-02	9.80E-03	1.00E-02	1.77E-03	1.77E-03	1.40E-02	5.87E-03	1.84E-03
3	1.00E-03	9.72E-05	9.83E-05	1.78E-05	1.77E-05	1.38E-04	5.75E-05	1.85E-05
4	1.00E-04	9.72E-07	9.83E-07	1.78E-07	1.78E-07	1.38E-06	5.74E-07	1.85E-07
5	1.00E-05	9.72E-09	9.83E-09	1.78E-09	1.78E-09	1.38E-08	5.74E-09	1.85E-09
6	1.00E-06	9.72E-11	9.84E-11	1.78E-11	1.78E-11	1.38E-10	5.74E-11	1.85E-11
7	1.00E-07	9.62E-13	1.04E-12	1.78E-13	1.78E-13	1.41E-12	5.60E-13	1.86E-13
8	1.00E-08	5.50E-14	1.90E-13	1.61E-15	7.48E-16	5.03E-14	8.53E-15	2.79E-15
9	1.00E-09	5.14E-14	2.01E-13	1.49E-15	9.86E-16	3.56E-14	8.25E-15	2.98E-15

CALC_USTAR

ii	ε	Δ/Δ_1			
		ALL	USTAR	Z0	CHARN
1	1.00E-01	1.00E+00	1.00E+00	1.00E+00	1.00E+00
2	1.00E-02	7.89E-03	1.11E-02	1.10E-02	2.12E-04
3	1.00E-03	7.87E-05	1.11E-04	1.11E-04	1.16E-06
4	1.00E-04	7.87E-07	1.11E-06	1.11E-06	1.06E-08
5	1.00E-05	7.87E-09	1.11E-08	1.11E-08	1.05E-10
6	1.00E-06	7.87E-11	1.11E-10	1.11E-10	1.03E-12
7	1.00E-07	7.83E-13	1.10E-12	1.07E-12	3.29E-14
8	1.00E-08	6.42E-15	6.57E-15	2.06E-15	6.19E-15
9	1.00E-09	3.29E-14	2.88E-14	6.74E-14	4.16E-14

CALC_USTAR Notes

To get acceptable test results, it was necessary that the magnitude of input parameter TAUW (representing the wind stress on the surface) be greater than zero. Otherwise, the values of Δ/Δ_1 for USTAR would not decrease as ε^2, instead remaining relatively constant.

W3SDS4

ii	ε	ALL	SRHS	DDIAG	BRLAMBDA
1	1.00E-01	1.00E+00	1.00E+00	1.00E+00	1.00E+00
2	1.00E-02	9.71E-03	9.71E-03	1.00E-02	1.04E-02
3	1.00E-03	9.68E-05	9.68E-05	1.00E-04	1.05E-04
4	1.00E-04	9.68E-07	9.68E-07	1.00E-06	1.05E-06
5	1.00E-05	9.68E-09	9.68E-09	1.00E-08	1.05E-08
6	1.00E-06	9.68E-11	9.68E-11	1.00E-10	1.04E-10
7	1.00E-07	9.65E-13	9.65E-13	9.82E-13	9.95E-12
8	1.00E-08	1.09E-14	1.09E-14	3.99E-14	9.87E-12
9	1.00E-09	9.75E-15	9.74E-15	2.13E-14	1.00E-11
10	1.00E-10	8.23E-15	8.22E-15	2.42E-14	1.10E-11

W3SDS4 notes

Output parameter WHITECAP_TL was not tested here, as the WHITECAP array is only used for statistical output (providing whitecap coverage, thickness, and moment at each location, along with mean breaking height) and not for any other computations in WW3.

6.2 Tests Completed with Minor Caveats (as noted)

W3SPR4:

* In W3SPR4 and W3SPR4_TL, the values of USDIR and USDIR_TL are simply set equal to the values of input parameters UDIR and UDIR_TL. When these input parameters are perturbed by ε, the output parameters are perturbed by the same factor. Thus, the parameter test value of Δ = (USDIR_P – USDIR) – USDIR_TL is essentially equal to (UDIR_P – UDIR) – UDIR_TL, and both quantities are nearly zero (to machine precision). In the actual computations, each difference turns out to be an extremely small number (i.e., O(1e-15)), so that the value of Δ, a ratio of these comparably small numbers, is close to 1.0.

** The values of EMEAN and EMEAN_TL are primarily computed linearly from the input values of wave action, A and A_TL, augmented a small amount by energy from a high frequency spectral tail. In our tests, the difference (EMEAN_P – EMEAN) – EMEAN_TL was again extremely small – essentially at the limit of machine precision – for all values of ε. Consequently, the ratio of Δ/Δ_1 was O(1.0) in all cases, as was the case for USDIR. An example of the values used to calculate Δ/Δ_1 at each iteration is provided in the third table below.

W3SPR4 – nonlinear output parameters

ii	ε	Δ/Δ_1									
		ALL	USTAR	FMEAN	FMEAN1	WNMEAN	CD	ZO	CHARN	FMEANWS	DLWMEAN
1	1.00E-01	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
2	1.00E-02	1.13E-02	1.05E-02	1.09E-02	1.09E-02	1.10E-02	1.13E-02	1.14E-02	1.16E-02	1.10E-02	9.49E-03
3	1.00E-03	1.15E-04	1.06E-04	1.10E-04	1.10E-04	1.11E-04	1.14E-04	1.15E-04	1.17E-04	1.11E-04	9.44E-05
4	1.00E-04	1.15E-06	1.06E-06	1.10E-06	1.10E-06	1.11E-06	1.15E-06	1.16E-06	1.18E-06	1.11E-06	9.44E-07
5	1.00E-05	1.15E-08	1.06E-08	1.10E-08	1.10E-08	1.11E-08	1.15E-08	1.16E-08	1.18E-08	1.11E-08	9.44E-09
6	1.00E-06	1.15E-10	1.06E-10	1.10E-10	1.10E-10	1.11E-10	1.15E-10	1.16E-10	1.18E-10	1.11E-10	9.56E-11
7	1.00E-07	1.15E-12	1.06E-12	6.38E-13	3.74E-13	1.46E-12	1.16E-12	1.14E-12	1.18E-12	9.40E-13	1.83E-12
8	1.00E-08	9.12E-15	8.79E-15	7.01E-13	7.01E-13	4.33E-13	9.75E-15	7.49E-14	1.88E-14	2.32E-13	1.30E-13
9	1.00E-09	4.38E-15	4.95E-15	1.02E-12	4.92E-13	2.44E-13	9.75E-16	7.64E-15	3.17E-15	1.94E-13	4.05E-13

W3SPR4 – linear outputs

ii	ε	Δ/Δ_1	
		USDIR*	**EMEAN****
1	1.00E-01	1.00E+00	1.00E+00
2	1.00E-02	2.31E+00	4.04E-01
3	1.00E-03	2.34E-01	4.52E-01
4	1.00E-04	7.77E-01	7.77E-02
5	1.00E-05	8.78E-01	1.61E+00
6	1.00E-06	3.11E+00	3.45E-01
7	1.00E-07	2.71E+00	9.61E-02
8	1.00E-08	5.29E-01	3.17E-01
9	1.00E-09	3.95E+00	9.55E-01

W3SPR4 – Expanded example of Δ/Δ_1 components (for Δ = |EMEAN_P – EMEAN1 – EMEAN_TL|)

ii	Δ	Δ_1	EMEAN_P	EMEAN1	EMEAN_TL
1.00E-01	7.11E-15	7.11E-15	9.6461049E+01	9.1733158E+01	4.7278913E+00
1.00E-02	1.92E-14	7.11E-15	9.2205947E+01	9.1733158E+01	4.7278913E-01
1.00E-03	3.77E-15	7.11E-15	9.1780436E+01	9.1733158E+01	4.7278913E-02
1.00E-04	2.09E-14	7.11E-15	9.1737885E+01	9.1733158E+01	4.7278913E-03
1.00E-05	9.20E-15	7.11E-15	9.1733630E+01	9.1733158E+01	4.7278913E-04
1.00E-06	1.23E-14	7.11E-15	9.1733205E+01	9.1733158E+01	4.7278913E-05
1.00E-07	1.97E-14	7.11E-15	9.1733162E+01	9.1733158E+01	4.7278913E-06
1.00E-08	5.49E-16	7.11E-15	9.1733158E+01	9.1733158E+01	4.7278913E-07
1.00E-09	2.42E-14	7.11E-15	9.1733158E+01	9.1733158E+01	4.7278913E-08

W3SBT1 and W3SIC4:

The "absolute difference" TL test based on Equation (8) is inappropriate for these subroutines, because in each case the primary output parameter (S) is essentially a linear function of the active input parameter (A). The secondary output parameter (D) is only a function of inputs and/or user-specified constants that are inactive in the operational model. As a result, $\Delta \approx 0$ to machine precision for all values of ε, which causes $\Delta/\Delta_1 \approx 1$ at each iteration. See examples for W3SBT1 in second table below. Note that both of these TL routines HAVE passed the "ratio" test based on Equation (7).

ii	ε	Δ/Δ_1	
		W3SBT1	**W3SIC4**
1	1.00E+00	1.00E+00	1.00E+00
2	1.00E-01	8.89E-01	9.49E-01
3	1.00E-02	9.18E-01	9.47E-01
4	1.00E-03	8.90E-01	9.63E-01
5	1.00E-04	9.08E-01	9.63E-01
6	1.00E-05	9.41E-01	8.84E-01
7	1.00E-06	9.03E-01	8.04E-01
8	1.00E-07	9.25E-01	8.34E-01
9	1.00E-08	9.06E-01	9.78E-01

W3SBT1 – Expanded example of Δ/Δ_1 components (for Δ = |S_P – S1 – S_TL|)

ii	**Δ**	**Δ_1**	**S_P**	**S1**	**S_TL**
1	3.61E-14	3.61E-14	5.2355882E+02	4.9879278E+02	2.4766034E+01
2	3.21E-14	3.61E-14	5.0126938E+02	4.9879278E+02	2.4766034E+00
3	3.31E-14	3.61E-14	4.9904044E+02	4.9879278E+02	2.4766034E-01
4	3.22E-14	3.61E-14	4.9881755E+02	4.9879278E+02	2.4766034E-02
5	3.28E-14	3.61E-14	4.9879526E+02	4.9879278E+02	2.4766034E-03
6	3.40E-14	3.61E-14	4.9879303E+02	4.9879278E+02	2.4766034E-04
7	3.26E-14	3.61E-14	4.9879281E+02	4.9879278E+02	2.4766034E-05
8	3.34E-14	3.61E-14	4.9879278E+02	4.9879278E+02	2.4766034E-06
9	3.27E-14	3.61E-14	4.9879278E+02	4.9879278E+02	2.4766034E-07

<u>W3SRCE and W3WAVE:</u>
These two higher-level routines both generally passed the "absolute difference" TL test based on Equation (8), with minor qualifications. In the case of W3SRCE_TL, several parameters were already treated in a linear fashion by the original nonlinear code, making this test inappropriate for them. For W3WAVE_TL, only values of the primary wave action parameter VA were tested.

W3SRCE – Most components (except PHICE, USDIR, TAUICE, VSIO, VDIO)

ii	ε	USTAR	USDIR	TAUOX	TAUOY	TAUWX	TAUWY	PHIAW	PHIOC	CHARN	TWS	PHIBBL	TAU ICE	WHITE CAP	TAU WIX	TAU WIY	TAU WNX	TAU WNY	TAU OCX	TAU OCY	WN MEAN
0	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
1	1.00E-01	1.47E-02	8.14E-03	1.07E-02	7.20E-03	1.03E-02	3.92E-03	2.32E-02	1.36E-02	2.12E+00	9.63E-03	5.30E-01	7.83E-03	1.09E-02	4.57E-02	5.75E-02	9.43E-03	1.04E-02	1.09E-02	1.00E-02	3.13E-01
2	1.00E-02	1.19E-04	7.18E-05	1.01E-04	5.97E-05	9.91E-05	3.90E-05	2.64E-04	1.16E-04	0.00E+00	9.37E-05	7.93E-05	6.90E-05	1.03E-04	6.45E-04	8.18E-04	9.23E-05	1.04E-04	1.35E-04	1.01E-04	9.87E-05
3	1.00E-03	1.19E-06	7.16E-07	1.01E-06	5.95E-07	9.92E-07	3.87E-07	2.64E-06	1.16E-06	0.00E+00	9.34E-07	7.52E-07	6.87E-07	1.03E-06	6.41E-06	8.13E-06	9.22E-07	1.04E-06	1.36E-06	1.01E-06	9.90E-07
4	1.00E-04	1.19E-08	7.16E-09	1.01E-08	5.95E-09	9.92E-09	3.87E-09	2.64E-08	1.16E-08	0.00E+00	7.54E-09	7.51E-09	6.87E-09	1.03E-08	6.41E-08	8.12E-08	9.22E-09	1.04E-08	1.36E-08	1.01E-08	9.90E-09
5	1.00E-05	1.18E-10	7.16E-11	1.01E-10	5.95E-11	9.92E-11	3.87E-11	2.64E-10	1.15E-10	0.00E+00	1.04E-09	7.51E-11	6.87E-11	1.03E-10	6.41E-10	8.12E-10	9.22E-11	1.04E-10	1.36E-10	1.01E-10	9.91E-11
6	1.00E-06	6.38E-13	7.01E-13	1.02E-12	5.87E-13	1.00E-12	4.12E-13	2.82E-12	3.44E-13	0.00E+00	2.00E-10	7.97E-13	6.77E-13	1.04E-12	6.41E-12	8.12E-12	9.01E-13	1.05E-12	1.22E-12	1.01E-12	9.43E-13
7	1.00E-07	3.95E-13	1.41E-14	8.47E-16	2.32E-14	1.41E-15	4.21E-14	3.42E-13	5.81E-13	0.00E+00	1.88E-09	3.99E-14	1.76E-14	1.25E-15	6.06E-14	7.70E-14	6.10E-15	1.61E-14	5.43E-14	1.47E-14	5.60E-14
8	1.00E-08	3.45E-13	1.41E-15	6.65E-15	5.73E-15	8.95E-15	4.88E-14	2.61E-13	5.70E-13	0.00E+00	1.28E-09	1.95E-14	4.11E-15	6.40E-15	2.13E-15	2.75E-15	7.34E-16	2.38E-14	1.59E-14	8.39E-15	3.22E-14
9	1.00E-09	1.18E-13	1.83E-14	3.77E-15	8.09E-15	1.13E-15	4.03E-14	1.22E-13	3.75E-13	0.00E+00	3.20E-10	3.96E-14	1.53E-14	2.62E-15	1.36E-15	1.30E-15	1.27E-14	4.47E-15	8.90E-15	1.04E-14	1.63E-14

W3WAVE – VA and VA_TL only

ii	ε	Δ/Δ_1
0	1.000000	1.000000
1	1.000001E-001	1.28E-002
2	1.000002E-002	1.26E-004
3	1.000002E-003	1.27E-006
4	1.000005E-004	1.48E-008
5	1.000006E-005	3.57E-010
6	1.000006E-006	2.67E-011
7	1.000007E-007	5.58E-012
8	1.000008E-008	3.68E-012