Gravity Wave Instability Dynamics at High Reynolds Numbers. Part I: Wave Field Evolution at Large Amplitudes and High Frequencies

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ABSTRACT

Direct numerical simulations are employed to examine gravity wave instability dynamics at a high intrinsic frequency, wave amplitudes both above and below nominal convective instability, and a Reynolds number sufficiently high to allow a fully developed turbulence spectrum. Assumptions include no mean shear, uniform stratification, and a monochromatic gravity wave to isolate fluxes due to gravity wave and turbulence structures from those arising from environmental shears or varying wave amplitudes. The results reveal strong wave breaking for both wave amplitudes, severe primary wave amplitude reductions within $\tau/2$ wave periods, an extended turbulence inertial range, significant excitation of additional wave motions exhibiting upward and downward propagation, and a net positive vertical potential temperature flux due to the primary wave motion, with secondary waves and turbulence contributing variable and negative potential temperature fluxes, respectively. Turbulence maximizes within $-\tau$ buoyancy period of the onset of breaking, arises almost entirely owing to shear production, and decays rapidly following primary wave amplitude decay. Secondary waves are excited by wave–wave interactions and the turbulence dynamics accompanying wave breaking; they typically have lower frequencies and smaller momentum fluxes than the primary wave following breaking.

1. Introduction

Internal gravity waves (GWs) and their instability processes are now widely recognized to play a variety of central roles in atmospheric dynamics extending from the earth’s surface into the thermosphere. GWs transport energy and momentum from sources in the lower and middle atmosphere, and the instability processes that accompany their propagation and amplitude increase with decreasing atmospheric density are responsible for the divergence of these energy and momentum fluxes at higher altitudes. These, in turn, drive various wave–wave and wave–mean flow interactions, the wave-induced residual circulation, and the mean transport accompanying this circulation. Turbulence due to GW breaking results in additional mixing and transport of heat, momentum, and constituents. These dynamics, and the motivations for and attempts to parameterize them, are reviewed in much greater detail by Fritts and Alexander (2003), Kim et al. (2003), and Fritts et al. (2006).

Initial studies of GW energy and momentum flux divergence and their effects on the large-scale circulation and structure employed linear theory to describe GW propagation and parameterize dissipation effects (Holton 1982, 1983; Garcia and Solomon 1985). These provided a basic understanding of the gross effects of GWs on the mean atmospheric circulation and structure. More advanced parameterization efforts attempted to account for broad GW spectra, nonlinearity, and filtering by mean and large-scale wind fields (see Fritts and Alexander 2003; Kim et al. 2003), and these efforts have met with additional successes, for example, in applications to the quasi-biennial oscillation (QBO) and semi-annual oscillation (SAO) at equatorial latitudes and to tidal fields at higher altitudes (Scaife et al. 2002; Medvedev and Klaassen 2001; Manson et al. 2002). However, they remain less robust in 1) characterizing the effects of GW interactions and instability for momentum transport and spectral evolution, 2) describing GW–tidal interactions in a consistent manner (and varying mean environments), and 3) accounting for secondary GW sources and GW penetration to much

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higher altitudes. Thus, to further advance the parameterization of GW effects throughout the atmosphere, a more complete understanding of the full range of GW interactions, instability, and effects is badly needed.

The drivers underlying GW effects are the nonlinear dynamics accounting for GW instability, exchanges of energy among scales, turbulent dissipation, and the energy and momentum flux convergence that results. These have been the subject of many studies employing theoretical, numerical, laboratory, and observational methods. At smaller GW amplitudes, these dynamics manifest as systematic exchanges of energy among GWs exhibiting weak “resonant” interactions (Klostermeyer 1991; Vanneste 1995; Sonmor and Klaassen 1997) that are believed not to impact GW momentum transport. At larger amplitudes, however, these instabilities lead to vigorous GW breaking, turbulence, spectral energy transfers, and divergent momentum fluxes that play the prominent roles in middle atmosphere dynamics noted above (Fritts 1984; Dunkerton 1987, 1989; Andreassen et al. 1998; Fritts et al. 1998, 2003, 2006; Lombard and Riley 1996; Sonmor and Klaassen 1997; Fritts and Alexander 2003).

Importantly, turbulence generation and GW dissipation may arise at small primary wave amplitudes as a result of subsequent wave superposition and/or wave–wave interactions (Fritts et al. 2006), while resonant interactions also play a role at large wave amplitudes, leading readily to turbulent dissipation (Thorpe 1994). Indeed, the instabilities occurring at large wave amplitudes are now understood to be finite-amplitude manifestations of the resonant interactions at smaller amplitudes (Sonmor and Klaassen 1997). More recent applications of optimal perturbation theory or singular-value analysis, pioneered elsewhere (Farrell and Ioannou 1996a,b), have demonstrated the importance of the lack of orthogonal eigenvectors in sheared environments for the growth and structure of transient perturbations in applications to GW instability (Achatz 2005, 2006, 2007; Achatz and Schmitz 2006a,b). Instability dynamics also impose both mean and spatially and temporally localized flux convergence that forces the zonal mean circulation and excites additional GWs at higher altitudes (Vadas and Fritts 2001, 2002; Fritts et al. 2002). Despite the significant advances noted above, we remain far short of a sufficiently complete understanding of GW interaction and instability dynamics to allow their more quantitative description and parameterization in large-scale research, numerical weather prediction, climate, and general circulation models. Arguably, such an understanding can only be obtained by high-resolution numerical simulations allowing the full range of GW instability dynamics and complete analyses of the resulting flows. While important progress has been made over the past decade, we remain far short of the Reynolds numbers needed to allow a full characterization of these dynamics in the mesosphere and lower thermosphere (MLT) and even further from the Reynolds numbers representative of the lower atmosphere. Studies at high Reynolds numbers are essential for several reasons: 1) large-scale responses to GW instability, including wave–wave interactions and local body forcing, depend on the spatial and temporal scales of instability; 2) competition between large-scale wave–wave interactions and local 3D instability plays a crucial role in GW breaking dynamics; and 3) 3D instability structures, scales, growth rates, and nonlinear evolution are highly dependent on Reynolds number for a wide range of GW amplitudes and frequencies. Thus, large-scale consequences of GW instability depend on the small-scale details to a degree that should not be discounted.

Until the past decade, computational resources allowed only 2D or limited 3D simulations of GW dynamics, and only the latter yielded glimpses of the instability dynamics accompanying GW breaking. Initial 3D studies by Andreassen et al. (1994) and Fritts et al. (1993, 1994, 1996) employed a low-resolution compressible code to study initial instability dynamics accompanying GW breaking in a shear flow. This required a parameterized description of turbulence dissipation at small scales, which was also employed in later higher-resolution studies describing the “twist” wave vortex dynamics driving the turbulence cascade (Andreassen et al. 1998; Fritts et al. 1998). A similar study of wave breaking in an oceanic context was performed by Winters and D’Asaro (1994). The initial instabilities in these studies took the form of streamwise-aligned (with largely spanwise wavenumber) counterrotating rolls that appeared to account for such features in MLT observations (Fritts et al. 1993).

Initial GW instability dynamics at more realistic Reynolds numbers employed a far more efficient pseudospectral code solving the Boussinesq Navier–Stokes equations employed initially for simulations of Kelvin–Helmholtz shear instability (Werne and Fritts 1999, 2001). This allowed more idealized GW instability studies (without mean shear) for a range of nondimensional GW amplitudes, $a = 0.5$ to $1.3$, an intrinsic frequency $\omega = N/3$, and Reynolds numbers $Re = 500$ to $3000$ (Fritts et al. 2003, 2006) with the larger Re values employed for smaller GW amplitudes. These studies revealed 1) substantial GW amplitude reductions (by factors of 2 to 3) for $a = 0.9$ and larger within $\sim 1$ to 2 GW periods following initial instability, 2) a tendency toward smaller spanwise instability scales at higher amplitudes and Re, 3) a preference for initial 2D wave–wave interactions at smaller initial GW amplitudes, 4) apparent competition between 2D wave–wave and 3D
local instability dynamics at all initial GW amplitudes, and 5) GW instability (and large-scale) dynamics that may vary considerably if initial instability pathways and scales are artificially constrained or precluded (by either the computational domain geometry or a low Re). While these simulations described turbulence spectra spanning some range of wavenumbers, the values of Re were nevertheless too limited to have confidence that they adequately characterized the various roles of turbulence within the overall dynamics of GW breaking and instability. There also remains a large range of GW frequencies, superpositions, and environments with mean or lower-frequency GW or tidal shears for which GW instability needs to be described in order to understand these dynamics more fully and address their parameterizations in large-scale models.

Our purposes in this and the companion paper by Fritts et al. (2009, hereafter Part II) are to begin to explore these GW instability dynamics at increasingly realistic Reynolds numbers. We will begin exploration of this wide parameter space by considering the simplest possible case. Specifically, we will study the instabilities of monochromatic GWs in an atmosphere at rest with constant stratification under the Boussinesq approximation. This will employ the efficient pseudospectral code used by Fritts et al. (2003, 2006), but at a significantly higher Reynolds number (∼10 times) that allows an extended inertial range of turbulence, greater confidence that high dissipation is not controlling the instability scales and wave breaking dynamics, and an assessment of turbulence structure, anisotropy, and implications for mixing and transport that was not possible previously.

Our paper is organized as follows: Section 2 describes our formulation of the problem, the numerical methods employed for these simulations, and their implementation on various supercomputer platforms. We describe in section 3 the qualitative evolution of the initial instability structures and the excitation of other GW motions at both primary GW amplitudes. Sections 4 and 5 provide quantitative discussions of the GW and turbulence structures arising for the two primary wave amplitudes. Our results are summarized and discussed in the context of earlier results in section 6. Part II employs these simulations to assess the turbulence structures, morphology, and anisotropy accompanying wave breaking for these cases.

2. Model formulation

a. Problem specification

As in previous studies by Fritts et al. (2003, 2006), we solve the nonlinear Navier–Stokes equations subject to the Boussinesq approximation in a Cartesian domain that is aligned along the phase of the primary GW. Non-dimensionalizing with respect to the GW vertical wavelength $\lambda_2$ and the buoyancy period, $T_b = 2\pi/\omega$, these equations may be written as

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mathbf{Ri} \mathbf{z} + \mathbf{Re}^{-1} \nabla^2 \mathbf{u},
\]

(1)

\[
\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = (\mathbf{Pr} \mathbf{Re})^{-1} \nabla^2 \theta,
\]

(2)

and

\[
\mathbf{V} \cdot \mathbf{u} = 0,
\]

(3)

where $\mathbf{u} = (u, v, w)$ is the total velocity vector, $p$ is pressure, and $\theta$ is total potential temperature. The bulk Richardson number relating the length and time scales of the Boussinesq approximation is $\mathbf{Ri} = N^2\lambda_2^2/U^2 = 4\pi^2$, the Reynolds number is $\mathbf{Re} = \lambda_2^2/\nu T_b = 10^4$, and the Prandtl number is $\mathbf{Pr} = \nu/\kappa$. The buoyancy frequency $N$ is defined by $N^2 = (g/\theta_0) d\theta/dz = g\beta/\theta_0$ in which $g$, $\theta_0$, and $\beta$ are gravity, mean potential temperature gradient, and kinematic viscosity and thermal diffusivity; and $\mathbf{z}$ is the unit vector in the vertical. The value of Re is appropriate for a GW in the mesosphere having $\lambda_2 \sim 3$ km and $\nu \sim 1$ m$^2$ s$^{-1}$. The linear, inviscid dispersion relation arising from these equations for general propagation directions is

\[
m^2 = (k^2 + l^2)(N^2/\omega^2 - 1),
\]

(4)

where $\omega = k_h c$ is the GW frequency, $k_h^2 = k^2 + l^2$ in which $k$ and $l$ are the wavenumbers along and normal to the direction of propagation of the primary GW, and $c$ is the GW horizontal phase speed.

The computational domain is displayed in Fig. 1, with streamwise, spanwise, and phase-normal directions ($x', y', z'$) defined along the GW group velocity, normal to the plane of the primary GW motions and opposite to the (downward) GW phase velocity, respectively. GW dynamics are described in this domain with components of gravity of $-g \sin \phi$ and $-g \cos \phi$ and potential temperature gradients of $\beta_1 = \beta \sin \phi$ and $\beta_2 = \beta \cos \phi$ in the $x'$ and $z'$ directions, respectively. A domain aligned along the GW phase offers several clear advantages for our current purposes: the evolving primary GW structure is trivial to assess; turbulence statistics can easily be evaluated at constant GW phase; and wave–wave interactions involving GWs having much lower frequencies are allowed that would be impossible to describe in a horizontally confined horizontal domain without restriction of these GWs to extremely small vertical scales. Tilted domains nevertheless impose their own allowed
mode interactions, and these are different, though arguably more general, than are enabled in a horizontal domain of similar dimensions.

We also employ a measure of GW amplitude expressed as $a = u'c/\beta = \left(d\theta'/dz\right)/\beta$, where $u'$ is the GW horizontal velocity amplitude, $d\theta'/dz$ represents the maximum gradient of the GW potential temperature perturbation, and $a = 1$ corresponds to insipient “convective” instability, at which the minimum “local” $\text{Ri} = 0$ and the maximum GW wind shear is $du'/dz = |\text{Ri}u'| = N$ (Sonmor and Klaassen 1997; Fritts et al. 2003, 2006).

Similarly, we refer throughout this paper and Part II to all wavenumber components as multiples of the gravest modes in each direction [e.g., $(1, 1, 1)$].

For the simulations discussed here, we assume monochromatic GWs having amplitudes of $a = 0.9$ and $1.1$, vertical and horizontal wavenumbers related by $mk = -3$, an intrinsic frequency $\omega \sim N/3.2$, no mean wind, constant stability $N$, a Reynolds number $\text{Re} = 10^4$, and a Prandtl number $\text{Pr} = 1$ so as to have comparable resolution requirements in the temperature and velocity fields. Both GW amplitudes are anticipated to be unstable based on linear stability considerations (Klostermeyer 1991; Lombard and Riley 1996; Sonmor and Klaassen 1997), but in observational studies (see Hecht 2004) there is often an artificial distinction drawn between GWs that are considered to be convectively “stable” with $a < 1$ and convectively “unstable” with $a > 1$.

Our chosen $\text{Re}$ is 10 times larger than the majority of our previous simulations and is intended to allow for an extended inertial range of turbulence at smaller spatial scales. The assumed Prandtl number differs slightly from the atmospheric value of $\text{Pr} \sim 0.7$, but we expect this difference to have an influence on the GW, instability, and turbulence structures only at the smallest spatial scales. Initial conditions for our simulations are a monochromatic GW with upward group velocity and downward phase progression and a white noise spectrum in the initial temperature field having a nondimensional rms amplitude of $10^{-5}$ (compared to a GW amplitude of $a = 0.9$ or $1.1$) that seeds initial instability structures.

To ensure that instability structures are not constrained by the extent of our periodic domain, we choose domain dimensions of $(X', Y', Z') = (3.4, 2.22, 1)$. This allows for multiple initial instability structures in both streamwise and spanwise directions for both GW amplitudes simulated. Our descriptions of the turbulence dynamics at this $\text{Re}$ require a maximum resolution of $(N_x, N_y, N_z) = (2400, 1600, 800)$ Fourier modes in the most turbulent phase of each evolution.

b. Computational methods and optimization

Our solution algorithm is pseudospectral and employs a Fourier series representation of the field variables in each direction, the third-order Runge–Kutta (RK3) method of Spalart et al. (1991) for time integration, a variable time step (due to varying flow velocities and model resolution) with a Courant–Friedrichs–Lewy (CFL) upper limit of 0.68, and a “2/3 rule” spectral truncation to avoid backscatter to larger spatial scales (Werne and Fritts 1999, 2001). Incompressibility is enforced via a two-streamfunction formulation, expressed as

$$ \mathbf{u} = \nabla \times \psi + \nabla \times \mathbf{v} \times \phi + \mathbf{U}_0 $$

in which streamfunctions $\psi = \psi(x, y, z)$ and $\phi = \phi(x, y, z)$ are defined by the vertical velocity and vertical vorticity fields, $\mathbf{U}_0 = U_0\mathbf{x} + V_0\mathbf{y}$ is a mean flow for general problems (but zero in our present application), and $x, y,$ and $z$ are unit vectors. Linear and nonlinear terms are treated implicitly and via transformation to, and multiplication in, physical space, respectively (Werne et al. 2005). To take full advantage of the cache architecture of the supercomputers on which these simulations were performed (a Cray T3E and XT3 and an SGI O3K at several DoD HPCMO supercomputer centers), FFTs are performed on contiguous data requiring data transposes to successively rotate the $x'$, $y'$, and $z'$ directions into the first array index and a global transpose requiring all-to-all communications among processors (Julien et al. 1996).

3. Overview of gravity wave breaking evolutions

a. Overview of GW breaking at $a = 1.1$

We can obtain a qualitative understanding of the wave breaking morphology, the initial instability scales and
structures, and the subsequent turbulence evolution from the 2D phase-aligned ($x', z'$) and spanwise ($y', z'$) cross sections of total vorticity magnitude. These are displayed at five times throughout the GW breaking evolution for $a = 1.1$ in Fig. 2, adjusted to remove the downward phase descent and display the images at a common GW phase. Here, bright regions are high vorticity owing to the primary and secondary GWs and initial instability structures at early times and are turbulent vortices at later times and smaller scales. Corresponding images of mean spanwise vorticity magnitude in the ($x', z'$) plane are displayed at the same times in the left column of Fig. 3 to illustrate the 2D ($l = 0$) evolution of the flow. Prior to strong instability dynamics and wave breaking ($t \sim 7–10$), the dominant instability structures occur at relatively small spanwise and vertical scales, are largely horizontally aligned (normal to $g$ with oblique or spanwise wavenumbers) rather than along the GW phase, and occur predominantly in the highly sheared portion of the upward phase of the primary GW. At the onset of strong instability, wave amplitude reductions, and turbulence generation ($t \sim 10$), the dominant instability scales have increased in the spanwise and vertical extent and now extend from the high shear region above, and throughout, the most convectively unstable phase of the primary GW (from the lower edge down through the upper half of the images in Fig. 2 at $t = 10$). Thereafter, initial instability dynamics give way to strong nonlinear turbulence dynamics ($t \sim 10–15$) and rapid development of a vigorous and extensive inertial range of turbulence. This causes the highest vorticity magnitudes to occur near the inner scale of the turbulence spectrum ($t \sim 12$). As turbulence decays, vorticity magnitudes indicate a superposition of structures, exhibiting alignment with the primary GW, and that are more nearly horizontal ($t \sim 15–30$). These will be seen below to be primarily 2D GWs (with $l = 0$, see the left column of Fig. 3) with predominant wavenumbers $\pm(1, 0, 1)$ and $\pm(1, 0, 2)$ that dominate the motion field at late times. The 2D and 3D dynamics accompanying GW breaking for $a = 1.1$ are explored more fully in section 4; the turbulence evolution is described in detail in Part II.

b. Overview of GW breaking at $a = 0.9$

The evolution of wave breaking and turbulence at $a = 0.9$ is similar in many respects to that described above for $a = 1.1$, despite the fact that the larger-amplitude GW is convectively unstable and the smaller-amplitude GW is convectively stable. Cross sections of total vorticity magnitude are shown for this case at five times in Fig. 4. As at $a = 1.1$, the primary instability involves 3D structures that are approximately horizontally aligned (with largely spanwise wavenumber) but now occur at larger scales and throughout the GW phase. They comprise counterrotating vortices that lead to largely spanwise and vertical undulations within the highly sheared regions of the primary GW immediately above and below the phase of lowest static stability: these structures occur at larger initial scales than seen at $a = 1.1$, and the 2D and 3D interactions accompanying instability lead to 2D GW and 3D turbulence evolutions that bear a close resemblance to those seen at $a = 1.1$. As for $a = 1.1$, the evolution of the 2D components of the motion field (with $l = 0$) is illustrated with streamwise cross sections of mean spanwise vorticity at the same times in the right column of Fig. 3. The major qualitative differences between these two breaking events are 1) delayed wave breaking by $\sim 10 T_b$ (or 3 GW periods), 2) larger instability scales, and 3) a more gradual wave breaking at $a = 0.9$ than at $a = 1.1$. These instability structures are displayed more clearly and discussed in detail in Part II.

c. Theoretical instability structures at $a = 1.1$ and 0.9

Linear instability theory applied to GWs seeks to describe the growth rates and expected modes of instability for specific GW amplitudes and intrinsic frequencies. In sheared flows, however, eigenmodes are typically not orthogonal and may exhibit a range of temporal behaviors. Linear analyses employing Floquet theory by Lombard and Riley (1996) and Sonmor and Klaassen (1997) have revealed a wide range of possible instability scales, orientations, and growth rates, often with several modes exhibiting competitive growth and suggesting sensitivity to initial conditions. Optimal perturbation, or singular vector, theory recognizes the potential for additional, transient, growth of perturbations arising from superposed nonorthogonal modes that may lead to nonlinear responses if seeded with sufficient amplitude (Achatz 2005, 2006, 2007; Achatz and Schmitz 2006a,b). However, optimal perturbations approach the most unstable eigenmode as optimization time increases, suggesting that linear Floquet theory should provide useful guidance to instability structure in the absence of strong initial perturbations. Indeed, Achatz (2005, 2006, 2007) noted, for GW parameters very similar to those considered here ($T = 2.92, a = 0.85$ and 1.04), that the spatial scales and orientations of optimal modes varied greatly with time, with smaller spatial scales and spanwise wavenumbers at early times and larger spatial scales and spanwise and oblique wavenumbers for the “global” optimal perturbations, apparently paralleling closely the evolutions displayed in Figs. 2 and 4.

To illustrate the range of instability character anticipated for the two cases considered here, we show in Fig. 5...
the eigenmode growth rates following the Lombard and Riley (1996) Floquet analysis. For \( a = 0.9 \), this analysis suggests possible streamwise, spanwise, and oblique alignments, with primary instabilities at wavenumbers \( k_i^2 + l_i^2 \sim 1 \) [with \( k_i \) and \( l_i \) the streamwise and spanwise wavenumbers nondimensionalized by the total wavenumber of the primary GW, following Lombard and Riley (1996)]. For \( a = 1.1 \), maximum growth rates approximately double, favored wavenumbers increase relative to \( a = 0.9 \) (now \( k_i^2 + l_i^2 \sim 1 \) and 4), and spanwise and oblique wavenumbers are favored over streamwise wavenumbers. These results suggest a range of possible instability orientations, with potentially very different instability character in each.

Examining the initial instability structures at early times in the \( a = 1.1 \) simulation shown in Fig. 2, we see that the dominant spanwise wavenumber decreases from \( l_i \sim 5 \) at \( t = 7 \) to \( l_i \sim 1 \) to 2 at \( t = 10 \) (corresponding to approximately two and five spanwise wavelengths, see also Fig. 1 of Part II). Thus, while early optimal perturbations appear to have very small scales and oblique alignments, the finite-amplitude instabilities appear to be

**Fig. 2.** Two-dimensional (left) streamwise-phase normal \((x', z')\) and (right) spanwise-phase normal \((y', z')\) cross sections of the wave breaking evolution in vorticity magnitude (white is high; black is zero) for \( a = 1.1 \) at times of 7, 10, 12, 15, and 30 (in units of \( T_b \)). All images are shown with the same GW phase, thus corrected for downward phase propagation, with the maximum upward motion within the wave field 1/4 of the domain depth from the top.
in close agreement with the predictions of Floquet theory (given the ratio of spanwise-to-phase normal extent of the computational domain of 2.22:1). Indeed, the appearance of both predicted scales and the ultimate dominance of $l_i \sim 1$ scales in the instability and turbulence fields (Fig. 2, $t = 10$ and 12; see also Fig. 1 of Part II), appears to confirm the slightly larger growth rate of the lower wavenumber mode, though these responses are well beyond the linear growth phase for either instability scale at $t = 10$.

The simulation for $a = 0.9$ is easier to evaluate in terms of linear theory as there is a clear spanwise wavenumber 2 response (corresponding to $l_i \sim 1$) hinted at in Fig. 4 at $t = 22$ (and seen clearly in Fig. 9 of Part II). There are also apparent influences of the oblique instability with $k_i \sim l_i$, suggested by the staggering of the finite-amplitude responses in the streamwise direction at alternating spanwise positions (Fig. 4, $t = 22$; also Fig. 9 of Part II). Hence, finite-amplitude instabilities for both $a = 1.1$ and 0.9 appear to be consistent with predictions of the linear theory of Lombard and Riley (1996), Sonmor and Klaassen (1997), and Achatz (2005, 2006, 2007).

Shown in the lower panels of Fig. 5 are the behaviors of the growth rates of the dominant modes with increasing $Re$. For $a = 0.9$, 2D ($l = 0$) and 3D ($l \neq 0$) modes are competitive at $Re \sim 10^3$, with 2D modes (streamwise wave–wave interactions) dominating for larger $Re$. At $a = 1.1$, in contrast, 2D modes only become important at much higher $Re$ that are more representative of GW instabilities at larger amplitudes and scales in the lower atmosphere.

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**Fig. 3.** As in Fig. 2 but showing the magnitude of the mean spanwise vorticity at each ($x', z'$) location for the simulations with (left) $a = 1.1$ and (right) $a = 0.9$ at the same times shown in Figs. 2 and 4. These fields display the presence of the 2D GWs more clearly than seen in Figs. 2 and 4, especially the primary GW and the influences of wavenumbers $\pm(1, 0, 1)$ and $\pm(1, 0, 2)$. The small-scale structures at intermediate times result from positive mean spanwise vorticity due to turbulent motions occurring primarily within the phase of the primary GW also having positive spanwise vorticity.
4. Gravity wave breaking and wave–wave interactions at $a = 1.1$

We describe here the implications of wave breaking for the primary GW, other GW motions arising in the breaking process, and the temporal evolutions of averaged variances and covariances of 2D (with spanwise wavenumber $l = 0$) and 3D motions (with $l \neq 0$). Note that velocities here are rotated from the computational domain and are either horizontal or vertical. We assume that the primary GW includes only velocities $(u, w)$ for the wavenumber $(0, 0, -1)$, and variances and covariances, defined as $\langle uu \rangle$ with subscripts denoting different fields that are averaged either 1) over a plane having constant primary GW phase or 2) over the full computational domain (as specified below) for either individual 2D modes $(k, l = 0, m)$ or 3D motions $(k, l \neq 0, m)$. Turbulence dynamics accompanying GW instability and the evolution of the large-scale GW field is described in Part II. Volumetric movies of these evolutions can be seen online (http://www.cora.nwra.com/dave/GWBmovies.html); these provide a much better understanding of the complex flow evolution than can be conveyed with a few images at specific times.

a. Evolution of 2D and 3D variances and covariances

The temporal evolution of the wave breaking simulation for $a = 1.1$, $\text{Re} = 10^4$, and other parameters defined
above is summarized in Fig. 6. Shown are domain-averaged variances and covariances of the velocity and potential temperature fluctuations for the primary GW and its opposite (having the same phase structure, but opposite propagation), with wavenumbers \((0, 0, 1)\) (light lines) and for all other motions (heavy lines). The variances (Fig. 6, upper left) show that the primary GW drops sharply in amplitude between \(t \approx 9\) and 13, consistent with the discussion above and our previous studies at much lower Re. The variance drops correspond to a decline in GW amplitude by a factor of \(\frac{1}{3}\), after which the variances for wavenumbers \((0, 0, 1)\), which are largely due to the primary GW, wavenumber \((0, 0, -1)\), remain fairly stable for many wave periods. The covariances for this mode pair exhibit oscillations at discrete periods persisting to late times, suggesting largely linear responses after breaking and turbulence decay (i.e., after \(t \approx 20\)). Because of its rapid variability, an expanded view of the vertical potential temperature fluxes during wave breaking is shown in the upper panel of Fig. 7.

The vertical flux of horizontal momentum (per unit mass) \((\omega \sqrt{\omega})\) exhibits a decay that mirrors that of the GW variances. Horizontal and vertical potential temperature fluxes by the primary GW (Figs. 6 and 7) exhibit sharp positive pulses during breaking (indicating an advance of the phase of the GW velocity perturbations relative to those of potential temperature) and weak oscillations at twice the primary GW frequency thereafter, suggesting excitation of wavenumber \((0, 0, 1)\) propagating opposite to the primary GW with a smaller amplitude. Covariances for modes \((0, 0, 1)\) containing the spanwise velocity \(\nu\) exhibit oscillations at the primary GW period. This suggests a superposition of GW motions having wavenumbers \((0, 0, 1)\) with a spanwise velocity having the same phase structure but no phase motion because the period of this oscillation would be zero or half the GW period if the \(\nu\) velocity field propagated with or opposed to the primary GW [see the small spanwise velocity variance for wavenumbers \((0, 0, 1)\) that cannot be associated with the primary GW and which must have zero frequency].
Variances for all other motions exhibit high variability during breaking, with significant magnitudes in all components that decay on a time scale of a few $T_b$ thereafter. The comparable magnitudes and rapid decay are indicative of strong turbulence discussed in connection with Fig. 2 above and Fig. 1 of Part II. Also seen are significant covariances, with the momentum flux for all other motions largely opposing that of the primary GW during breaking and strong turbulence. The other motions also yield negative potential temperature fluxes.
During breaking, largely offsetting the primary GW flux, with an oscillatory potential temperature flux of small amplitude extending to late times. The offsetting potential temperature fluxes between the primary GW and all other motions appear to suggest weak thermal transport and a large turbulence Prandtl number, as inferred in earlier theoretical studies. Both variances and covariances exhibit a range of periodicities after turbulence has largely subsided (after $t \sim 20$), suggesting excitation of larger-scale motions that exhibit largely linear dynamics at smaller amplitudes following wave breaking, but which continue to interact weakly to late times.

Simplifying somewhat, there are two general classes of motions excited during wave breaking. These include 1) largely 3D motions [having wavenumbers $(k, l \neq 0, m)$], which we will refer to as turbulence, that largely decay following wave breaking, and 2) identifiable and persistent 2D motions [wavenumbers $(k, l = 0, m)$; see Fig. 3] that also arise during wave breaking, but which generally persist or continue to grow in amplitude at later times and display specific periodicities. It is important to note, however, that there is also clear evidence of nonturbulent 3D motions ($l \neq 0$) that appear to satisfy the linear GW dispersion relation, Eq. (4), as well as 2D ($l = 0$) motions that clearly do not. Thus, Eq. (4), rather than spatial orientation, represents the best means of distinguishing GWs and turbulence in our simulations.

We now decompose those motions described by the heavy curves in Fig. 6 into 2D “GWs” and 3D “turbulence.” Although this distinction is not quantitative, it will be seen that it largely separates the early turbulent, and nonlinear, dynamics from the later, and largely linear, GW dynamics. These 2D and 3D fields are shown with light and heavy lines, respectively, in Fig. 8 with the vertical potential temperature fluxes during wave breaking displayed separately in the lower panel of Fig. 7. Referring to the 2D curves (the light curves in Figs. 7 and 8) first, we see that these motions make relatively smaller contributions to the variances and covariances during strong wave breaking, except for the 2D potential temperature flux, where 2D motions make the dominant contribution and 3D motions contribute little, if at all. However, 2D motions account for the large majority of variances and covariances and for nearly all of the oscillatory behavior at late times ($t > 40$; see Fig. 3). Indeed, there are a number of specific periodicities that suggest that the later flow is dominated by a small number of specific GW motions and superpositions, as well as continuing nonlinear interactions (see below). The 3D (heavy) curves generally exhibit rapid decay as turbulence subsides and essentially no discernable oscillatory behavior at late times. It is also noteworthy that the 3D motions account for the majority of the momentum flux and the horizontal potential temperature flux, but the 2D motions account for a majority of the vertical potential temperature flux during wave breaking. This suggests that the former accompany largely streamwise-aligned (spanwise wavenumber) motions at smaller scales at early stages of wave breaking (see Fig. 1 of Part II) and the latter are due primarily to 2D structures extracting energy from the coherent primary GW rather than to the specific regions of instability at its most unstable phase.

We can gain an appreciation of the excitation of other 2D and 3D motions by examining the equations that couple the various motions. Assuming, for simplicity, that dissipation is weak and the only significant source of energy for other motions at early times is the primary GW, the growth of energy in a mode with 3D wavenumber $k = (k, l, m)$ may be written as

$$
\delta E(k)/\delta t = -(ik/2)[u^*_i(k)u_i(k_{GW})u_i(k-k_{GW}) - u_i(k)u^*_i(k_{GW})u_i^*(k-k_{GW})] - (ik/2) \text{ Re} [\theta^*_i(k)\theta_i(k_{GW})\theta_i(k-k_{GW}) - \theta_i(k)\theta^*_i(k_{GW})\theta_i^*(k-k_{GW})],
$$

where $\theta_i(k)$ is the mean horizontal component of the velocity at wave number $i$. The growth of the 2D modes is given by

$$
\delta E(k)/\delta t = -(ik/2)[u^*_i(k)u_i(k_{GW})u_i(k-k_{GW}) - u_i(k)u^*_i(k_{GW})u_i^*(k-k_{GW})] - (ik/2) \text{ Re} [\theta^*_i(k)\theta_i(k_{GW})\theta_i(k-k_{GW}) - \theta_i(k)\theta^*_i(k_{GW})\theta_i^*(k-k_{GW})].
$$

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where $u_i(k)$ and $\theta_i(k)$ are Fourier coefficients of the component velocities and potential temperature for the interacting modes, the total energy in mode $k$ is

$$E(k) = [u_i^*(k) u_i(k) + \text{Ri} \theta^*(k) \theta(k)]/2,$$

$k_{GW}$ is the wavenumber of the primary GW, asterisks denote a complex conjugate, $k_j$ denote wavenumber components, and repeated indices imply summation. Frequencies for each mode $k = (k', l', m')$ arising via such interactions are dictated by Eq. (4) and are specified in terms of the initial wavenumber $(k', l', m')$ in the computational domain as $k = k' \cos \phi - m' \sin \phi$, $l = l'$, and $m = k' \sin \phi + m' \cos \phi$ in geophysical coordinates.
From Eq. (6), we see that the primary GW can excite other motions through interactions among the velocity or the potential temperature fields, resulting in wave-number pairs $k$ and $k_1 = k - k_{GW}$ that are either both 2D (with $l = 0$) or 3D (with $l \neq 0$). Resonant wave–wave interactions are those for which both $k_1 = k - k_{GW}$ and $\omega_1 = \omega - \omega_{GW}$ are simultaneously satisfied (Klostermeyer 1991; Müller et al. 1986). But strong interactions can also occur off resonance for sufficiently large wave amplitudes. As discussed further below, the motions that dominate the late-time solutions are primarily 2D (with $l = 0$) motions in the plane of the primary GW due to an obvious excitation of parallel (streamwise) motions by the primary GW. We also note that the interactions that excite other GW motions are constrained by our choice of the computational domain geometry. This causes the spectrum of excited motions to be much more strongly discretized than would be the case in either a larger model domain or the real atmosphere.

As noted above, 2D motions at late times exhibit a relatively small number of apparently discrete periods ranging from $\sim 1$ to $28 T_b$ (owing to the imposed discretization). Indeed, modes $\pm (1, 0, 1)$ and $\pm (1, 0, 2)$ (having periods of $\sim 28$ and $5.7 T_b$, respectively) appear to account for a majority of the total 2D variances (see Fig. 9), although modes $\pm (2, 0, 1)$ also contribute measurably to the 2D fields, especially at earlier times. The variances not accounted for by these three wave-number pairs are relatively small and appear to include variances from a significant number of additional 2D modes at smaller amplitudes. To further quantify these contributions and their potential interactions, the frequency spectra of the domain-averaged variances and covariances for the primary GW and its opposite, $\pm (0, 0, 1)$, and for modes $\pm (1, 0, 1)$ and $\pm (1, 0, 2)$ for the interval from $t = 24–80$, are displayed in Fig. 10. To avoid aliasing, we also employ linear trend removal and Welch windowing of the resulting time series. A summary of the dominant periods observed is provided in Table 1. Periods expected based on sum and difference frequencies involving interactions of the gravest modes are listed for reference in Table 2. While these motions make appreciable contributions to the variances and covariances, they are not apparent in the images in Figs. 2 and 3 because larger-scale (small $|m|!$) motions (including the primary GW) contribute much less to total (or mean spanwise) vorticity and its gradients than motions having smaller amplitudes but much larger $|m|!$.

These data suggest three classes of responses, based on the correlations between different GW perturbations and propagation directions. Dominant periods are closely correlated among 1) $u$, $w$, and $\theta$ variances and the vertical flux of horizontal momentum, $\langle uw \rangle$, 2) streamwise and vertical potential temperature fluxes, $\langle u\theta \rangle$ and $\langle w\theta \rangle$, and 3) momentum and potential temperature fluxes involving the spanwise velocity, $\langle u\nu \rangle$, $\langle w\nu \rangle$, and $\langle \theta\nu \rangle$. Modes $\pm (1, 0, 1)$ exhibit class-1 and -2 modulations at $T \sim 14$, with much smaller modulations at $T \sim 1.6–2.2$ not seen in Fig. 10. Class-3 modulations involving $\nu$ occur at $T \sim 28$ due to the lack of phase progression of the spanwise motions, hence a modulation at the mode $\pm (1, 0, 1)$, and at $T \sim 2.8–3.6$ due to interactions with the primary GW, which also contributed to its sideband modulations noted above (see the left panels of Fig. 10 and Table 1). Modes $\pm (1, 0, 2)$ exhibit class-1 and -2 modulations at $T \sim 2.3$ and class-3 modulations involving $\nu$ at $T \sim 3.6$ and $\sim 5–7$. The latter imply interactions with the primary GW and possibly also mode $\pm (1, 0, 1)$. The specific mode interaction accounting for the period $T \sim 2.3$ was not diagnosed as this mode contributes very little to the 2D motion field. However, it is suggestively close to the first harmonic of the higher frequency product resulting from the interaction with the motion field following primary GW breaking, and we should expect that the spectrum of GW motions would be even broader if not constrained by the computational domain geometry. But those motions diagnosed above clearly account for most of the late-time behavior, and further discussion of much smaller contributions seems unwarranted.

b. Competition between wave–wave interaction and turbulence dynamics

Given the various 2D and 3D dynamics contributing to GW breaking discussed above, we also examine the competition between the largely 2D wave–wave interactions and the 3D instability and turbulence dynamics driving the energy cascade. Specifically, which dynamics contribute primarily to reduction of the primary GW amplitude, and do 3D instability and turbulence dynamics impact the excitation and evolution of 2D motions at late times?

To explore this, we perform a series of 2D simulations to evaluate the efficiency of 2D GW excitation in the presence and absence of 3D instabilities. Strictly 2D simulations are performed with three initial 2D phase specifications among the primary GW and all other possible modes having amplitudes within the noise spectrum, defined as 1) random initial phases, 2) uniform initial phase at one $(x', z')$ location, and 3) identical 2D phases between the 2D and 3D simulations. Comparisons of the variations of the variances of horizontal $(x)$ velocity for the primary GW and the gravest modes noted above,
as displayed in Fig. 11. As expected, the primary GW (heavy solid line) decays most rapidly when it is subjected to the full range of possible instability dynamics. Primary GW decay is delayed an additional \(-5-7 \, T_b\) when 3D instability and turbulence dynamics are suppressed, but the decay is to a smaller final amplitude when due only to 2D wave–wave interactions, as noted previously by Fritts et al. (2006) for smaller initial GW amplitudes. Comparing the evolutions of modes \(\pm (1, 0, 1)\) and \(\pm (1, 0, 2)\), we see that
these modes achieve substantially larger variances in the absence of 3D dynamics. They also exhibit the same periodicities discussed above, although modes $\pm (1, 0, 2)$ exhibit a much larger transient response than in the presence of 3D dynamics. What is perhaps surprising is that these other modes, especially $6 \pm (1, 0, 1)$, display a more rapid initial growth in the presence of 3D instability and turbulence processes than in their absence, suggesting that 3D motions act to enhance 2D energy transfers, despite also competing with them for primary GW energy during wave breaking. At all times, the lack of 3D turbulent energy dissipation in the 2D evolutions ensures that there is more energy available for excitation of 2D modes thereafter. We also note a tendency in all the 2D simulations for modes $\pm (1, 0, 1)$ to apparently grow at the expense of modes $\pm (1, 0, 2)$ at late stages in each evolution.

5. Gravity wave breaking and wave–wave interactions at $a = 0.9$

Our discussion here parallels that of section 4 for $a = 0.9$, primarily through comparisons of the results at the two GW amplitudes. As above, the corresponding evolution and character of the turbulence spectrum accompanying wave breaking at $a = 0.9$ is described in Part II.

a. Evolution of 2D and 3D variances and covariances

The similarities between the wave breaking simulations at $a = 1.1$ and 0.9 also extend to the other fields displayed for $a = 1.1$ in Figs. 6–11. Here we limit our focus to comparisons between the two rather than a repetition of the full discussion in section 4 above for $a = 0.9$. Comparing first the variances and covariances of the primary GW [and wavenumber $(0, 0, 1)$] with all other flow components in Figs. 6 and 12, we see that the evolutions are very similar with the primary differences being 1) a longer turbulence decay time (by a factor of $\sim 2$), 2) generally smaller variances and covariances in the primary GW at $a = 0.9$, 3) smaller but comparable covariances in the remaining motion field at $a = 0.9$, and 4) much more oscillatory response in the streamwise and vertical potential temperature fluxes than at $a = 1.1$. In other respects, the dominant oscillations and their modulation periods are essentially identical in the two simulations following the decay of large turbulence energy (after $t \sim 40$ for $a = 0.9$).

As at $a = 1.1$, the vertical flux of horizontal momentum (per unit mass), $(u w)$, exhibits a decay that mirrors that of the GW variances. Streamwise and vertical potential temperature fluxes exhibit much more variability during and after wave breaking at $a = 0.9$, and the vertical fluxes are displayed in the upper panel of Fig. 13 to illustrate this behavior more clearly. GW potential temperature fluxes exhibit positive pulses lasting several $T_b$ and then undergo large-amplitude oscillations at several periods that continue to late times. The positive fluxes accompanying wave breaking are of similar duration to those at $a = 1.1$, but the magnitudes are

### TABLE 1. Dominant periods seen in the variances and covariances of the gravest modes at $a = 1.1$.

<table>
<thead>
<tr>
<th>Dominant 2D periods (in $T_b$)</th>
<th>$(0, 0, -1)$</th>
<th>$(1, 0, 1)$</th>
<th>$(1, 0, 2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u, w, \theta$ variances; $uw$</td>
<td>1.6, 2.0, 9, 14, 28</td>
<td>14</td>
<td>2.3</td>
</tr>
<tr>
<td>$u\theta, w\theta$</td>
<td>1.6, 2.0, 2.2</td>
<td>14</td>
<td>2.3</td>
</tr>
<tr>
<td>$uw, uw, w\theta$</td>
<td>2.8, 3.2, 3.6</td>
<td>2.8, 3.6, 28</td>
<td>3.6, 5–7</td>
</tr>
</tbody>
</table>
smaller by ~5 times. Oscillations in the fluxes following wave breaking are larger in magnitude than at \( a = 1.1 \), despite the much smaller initial positive fluxes. The enhanced oscillations of GW flux at late times suggest excitation of wavenumber \((0, 0, 1)\) propagating opposite to the primary GW with a larger relative amplitude than at \( a = 1.1 \). Fluxes due to all other motions are very similar to those at \( a = 1.1 \), with small initial positive values as wave breaking begins, larger negative fluxes that partially offset the positive fluxes due to the primary GW during breaking, and smaller magnitudes at early times. Following wave breaking, the oscillatory fluxes due to all other motions are larger at \( a = 0.9 \) than at \( a = 1.1 \). The vertical potential temperature flux of the primary GW is offset by that due to other motions to a smaller degree at \( a = 0.9 \) than at \( a = 1.1 \).

Primary GW covariances containing \( \nu \) also exhibit oscillations at the primary GW period but are now modulated at a period of ~28 \( T_b \), suggesting a stronger influence of secondary GWs at wavenumbers \( \pm (1, 0, 1) \). Variances for all other motions also exhibit sharp spikes during breaking and decay on a timescale approximately twice as long as at \( a = 1.1 \), consistent with the slower decay of the primary GW amplitude and more gradual generation of turbulence at \( a = 0.9 \) noted above. Thereafter, we see the same oscillation periods noted at \( a = 1.1 \), but now with larger amplitudes at ~14 and 28 \( T_b \) periods. In other respects, the two simulations are very similar, including an earlier, energetic turbulence phase accompanying wave breaking and a later phase comprising identifiable and persistent 2D motions [wavenumbers \( (k, l = 0, m) \)] that persist to late times.

We now decompose those motions described by the heavy curves in Fig. 12 into 2D GWs and 3D turbulence. These 2D and 3D fields are shown in Fig. 14 with light and heavy lines, respectively. As at \( a = 1.1 \), we display the vertical potential temperature fluxes for these 2D and 3D motions separately in the lower panel of Fig. 13. As at \( a = 1.1 \), this separation of 2D and 3D motions largely distinguishes the earlier, and more turbulent, nonlinear dynamics (which largely decay with time) from the later, largely linear GW dynamics (which exhibit coherent structures and long-term, systematic variations—see Fig. 3). It also demonstrates, as for \( a = 1.1 \), that the 2D wave motions, rather than 3D turbulence, account for the majority of the negative vertical potential temperature flux, compensating that due to the primary GW during breaking, with the opposite being the case for the streamwise potential temperature flux. To understand the composition of the 2D fields more fully, we also display them separately for modes \( \pm (1, 0, 1) \) and \( \pm (1, 0, 2) \) in Fig. 15. As noted above, the 2D oscillations, especially wavenumbers \( \pm (1, 0, 1) \), account for large fractions of a number of the variances and covariances. Wavenumbers \( \pm (1, 0, 1) \) are also larger in amplitude at \( a = 0.9 \) than at \( a = 1.1 \). As at \( a = 1.1 \), however, the amplitude oscillations in the 2D variances and the streamwise and vertical potential temperature fluxes, \( \langle w\theta \rangle \) and \( \langle u\theta \rangle \), suggest a beat between the upward and downward propagating components in wavenumbers \( \pm (1, 0, 1) \) and at other wavenumbers having higher frequencies. Also similar are the oscillations seen in the covariances \( \langle u\theta \rangle \) and \( \langle uv \rangle \), primarily at a period of ~28

<table>
<thead>
<tr>
<th>2D mode interactions</th>
<th>( (0, 0, -1) \pm (1, 0, 1) )</th>
<th>( (0, 0, -1) \pm (1, 0, 2) )</th>
<th>( (0, 0, -1) \pm (1, 0, -1) )</th>
<th>( (0, 0, -1) \pm (1, 0, 0) )</th>
<th>( (0, 0, -1) \pm (0, 0, -2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_b )</td>
<td>2.86</td>
<td>3.6</td>
<td>2.0</td>
<td>7.3</td>
<td>1.1</td>
</tr>
</tbody>
</table>

Table 2. Dominant periods based on sum and difference frequencies of the gravest 2D modes.

Fig. 11. Excitation of the gravest 2D wave modes for \( a = 1.1 \) by 3D breaking dynamics (heavy solid) and by 2D wave–wave interactions with random initial phase (solid), uniform phase at one streamwise location (long dashed), and the same phase as in the 3D simulation (short dashed). Shown here are the variances of (top) the initial GW with wavenumber and its opposite \( \pm (0, 0, 1) \), (middle) modes \( \pm (1, 0, 1) \), and (bottom) \( \pm (1, 0, 2) \).
$T_b$. Higher frequencies are seen in these latter covariances than at $a = 1.1$, however, and these will be examined in greater detail below. Finally, we note a low-frequency modulation of the covariance $\langle vw \rangle$ in the 3D field that was not observed at $a = 1.1$ and cannot be attributed to any defined 2D motions (with $l = 0$). This appears to be a signature of the excitation of the wave-numbers $\pm(1, \pm1, 1)$, which are 3D GWs having oblique propagation and a period of $\sim 33 T_b$.

As noted for $a = 1.1$, 2D motions occurring for $a = 0.9$ at late times also exhibit a small number of discrete periods, with modes $\pm(1, 0, 1)$ and $\pm(1, 0, 2)$ accounting for a majority of the total 2D variances (Fig. 15). Compared to the results for $a = 1.1$, modes $\pm(1, 0, 1)$ for $a = 0.9$ make significantly larger contributions to all variances, with spanwise variance not due to GWs. Higher-order 2D motions contribute comparably or more significantly to all variances at $a = 0.9$ relative to $a = 1.1$. 

**FIG. 12.** As in Fig. 6 but for $a = 0.9$. 
Vertical velocity variance exhibits a large background and weak modulations at periods of \( \sim 1-15 \) \( T_b \); vertical momentum flux exhibits large oscillations at periods of \( \sim 5-15 \) \( T_b \); and vertical potential temperature flux exhibits variability primarily at periods of \( \sim 1-2 \) \( T_b \). In all cases, these quasiperiodic oscillations are significantly larger for \( a = 0.9 \) than for \( a = 1.1 \).

Frequency spectra of these variations for the interval from 36 to 120 are displayed in Fig. 16, again employing linear trend removal and Welch windowing. As for \( a = 1.1 \), these responses appear to organize in three classes, with fairly discrete frequency bands observed for each. Again, dominant periods are closely correlated among 1) \( u \), \( w \), and \( \theta \) variances and the vertical flux of horizontal momentum, \( \langle uw \rangle \), 2) streamwise and vertical potential temperature fluxes, \( \langle u\theta \rangle \) and \( \langle w\theta \rangle \), and 3) momentum and potential temperature fluxes involving the spanwise velocity, \( \langle uw \rangle, \langle pw \rangle, \) and \( \langle u\theta \rangle \). We cannot see evidence of the enhanced responses seen at \( a = 0.9 \) because the spectra have been normalized. However, the bands of peak responses are essentially the same for the two simulations, indicating that the wave–wave interactions generating these periodicities are the same, the only differences being the amplitudes of the interacting modes. Again, the primary GW exhibits class-1 responses at periods of \( \sim 1.6-2.3 \) and \( \sim 8 \) and greater, class-2 responses primarily at periods of \( \sim 1.6-2.3 \), and class-3 responses at periods of \( \sim 2.4-4.2 \) and 28. Modes \( \pm (1, 0, 1) \) exhibit class-1 and -2 responses at periods of \( \sim 14-20 \) and class-3 responses primarily at periods of \( \sim 28 \). Finally, modes \( \pm (1, 0, 2) \) exhibit class-1 responses at periods of \( \sim 1.8-2.7 \) and \( \sim 12 \) and greater, class-2 responses at periods of \( \sim 1.8-2.7 \), and class-3 responses at periods of \( \sim 1.8-28 \). The increased spectral structure seen in Fig. 16 is a consequence of the greater temporal extent of the spectral computations for \( a = 0.9 \).

b. Competition between wave–wave interaction and turbulence dynamics

We now compare the 3D wave breaking evolution for \( a = 0.9 \) both with restricted 2D simulations at \( a = 0.9 \) and via the same 3D versus 2D comparisons discussed above for \( a = 1.1 \). Comparing first the 3D and the 2D evolutions for \( a = 0.9 \) (see the top panel in Fig. 17), we see that the 3D evolution experiences primary GW amplitude reductions nearly simultaneously with two of the 2D simulations and slightly earlier than the third. In fact, the 2D simulation initiated with the same 2D phases as the 3D simulation exhibits more rapid amplitude growth of the resulting mode pairs than even the 3D simulation. In other respects, the simulations parallel those seen at \( a = 1.1 \), with 1) greater total GW amplitude reductions in 2D than in 3D, 2) significant growth and temporal evolution of the other two mode pairs achieving comparable or larger amplitudes than in 3D, and 3) faster relative growth, but slower total growth, of modes \( \pm (1, 0, 1) \) relative to modes \( \pm (1, 0, 2) \) at later times.

The main difference between the simulations at \( a = 0.9 \) and 1.1 is the apparently different role of 3D instabilities, which enhance GW amplitude reductions relative to 2D simulations at \( a = 1.1 \) but not obviously at \( a = 0.9 \). In general, of course, we expect this to be the case. But other factors may also play a role here. These include possibly different 2D GW phase influences, as the instabilities arise at different times at the two GW amplitudes, and potentially different instability roles, as instabilities with spanwise or oblique wavenumbers are favored at \( a = 1.1 \), while instabilities having streamwise wavenumbers spanning a wide range of scales, and perhaps enhancing 2D wave–wave interactions, are at least as competitive for \( a = 0.9 \).

6. Summary and conclusions

We performed high-resolution simulations of GW breaking for waves having an intrinsic frequency \( \omega \sim N/3.2 \) and amplitudes of \( a = 0.9 \) and 1.1. Our simulations employed a spectral code yielding high accuracy and resolution, allowing us to achieve a Reynolds number \( Re = 10^6 \) and a vigorous and well-developed inertial range of turbulence. The computational domain was chosen...
to ensure sensitivity to the dominant instability scales accompanying the transition to turbulence and allow the largest possible extent of the turbulence spectrum. These foci, and the periodic boundary conditions, required that the computational domain be as small as possible and led to our choice of a domain having dimensions \((X', Y', Z') = (3.4, 2.22, 1) \lambda\). The small computational domain implied a significant discretization of the larger-scale modes that can be described relative to what would occur without such a constraint. While we have not assessed this constraint in detail, wave–wave interactions occurring in much larger domains at smaller \(Re\) suggest that smaller domains exhibit similar interactions.

Wave breaking for initial wave amplitudes of \(a = 0.9\) and 1.1 exhibit strong similarities and significant differences. Similarities among the two simulations discussed here include

![Graphs showing various turbulence spectra and wave–wave interactions](image-url)

**Fig. 14.** As in Fig. 8 but for \(a = 0.9\).
1) strong GW breaking and wave amplitude reductions accompanying instability, turbulence generation, and wave–wave interactions;

2) opposite potential temperature fluxes for the initial GW (positive) and all other motions (negative) during wave breaking;

3) common periods of the 2D modes in the wave field excited through wave–wave interactions, primarily modes \((1, 0, 1)\) and \((1, 0, 2)\), including apparent beats between modes having opposite propagation and common modulation periods;

Fig. 15. As in Fig. 9 but for \(a = 0.9\). The totals for all 2D motions shown previously in Fig. 11 are reproduced as green lines for comparison.
4) successive positive and negative pulses of the vertical turbulence momentum flux \( \langle u'w' \rangle \) in both the 2D and 3D fields excited by wave breaking;  
5) initial GW amplitude reductions that are larger accompanying wave–wave interactions in 2D simulations than when 3D dynamics are enabled; and  
6) corresponding secondary GW excitation that is larger in the absence of 3D dynamics.

Important or significant differences between the simulations for \( a = 0.9 \) and 1.1 include

1) differences in the initial instability spanwise scales, with larger structures occurring for \( a = 0.9 \) than for \( a = 1.1 \) by a factor of \( \sim 2 \) (as anticipated by Floquet theory);  
2) delayed instability onset and longer duration of GW breaking (\( \sim 2 \) GW periods) for \( a = 0.9 \) relative to that for \( a = 1.1 \) (\( \sim 1 \) GW period);  
3) much larger potential temperature fluxes during GW breaking for \( a = 1.1 \), for which the initial GW was convectively overturning, than for \( a = 0.9 \), which was not; and  
4) comparable, though slightly smaller, variances and covariances of the 2D motion field during and after wave breaking for \( a = 0.9 \).

Summarizing the above similarities and differences, wave breaking is vigorous for GWs having a relatively high frequency of \( \omega \sim N/3.2 \) and a large amplitude, whether the GW is convectively unstable or convectively stable. GW amplitude reductions accompanying breaking are large but consistent with our earlier, lower-Re studies (Fritts et al. 2003, 2006) and the 2½-D computations by Achatz (2006, 2007). Wave breaking and turbulence generation occupy \( \sim 1–2 \) GW periods at this GW frequency, with the more unstable (larger amplitude) initial GW exhibiting more rapid breaking and more intense turbulence. In many respects, these results also closely parallel our earlier, lower-Re compressible GW breaking simulations in a mean shear (Andreassen et al. 1994, 1998; Fritts et al. 1994, 1996, 1998), including common instability characteristics and GW responses.

Wave breaking is accompanied by significant wave–wave interactions that excite primarily lower-frequency GWs that dominate the late-time motion field after turbulence has largely subsided. We expect, based on earlier laboratory studies (Thorpe 1994) and other simulations...
not discussed here, that these general results, and especially the occurrence of both wave breaking and wave–wave interactions, will also apply to such dynamics when the resulting motions are not constrained by a small computational domain. The implications of these results are that wave breaking at relatively large GW amplitudes is likely to be episodic and locally strong (because of the large amplitudes at which it is initiated and the much smaller amplitudes to which it collapses), rather than slow and systematic, and that both turbulent dissipation and wave–wave interactions must be accounted for in any significantly improved parameterization of GW effects in models that cannot resolve these dynamics explicitly.

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