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Scalable Modeling of Acoustic-Gravity Wave Interactions, Coupling and Observables from Surface to Space

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Abstract:

Numerical simulations of acoustic-gravity wave (AGW) processes in the deep atmosphere are complicated by the wide range of scales involved. Small-to-medium-scale AGWs, with wavelengths ~10s-100s km and periods of several-to-tens of minutes, interact with structure dynamics ranging from sub-km to global scales. It remains infeasible to capture all relevant scales and processes in single domains, e.g., to comprehensively resolve turbulent eddies, radiation of secondary AGWs into the thermosphere, and interactions with tides (e.g., *Heale et al.*, JGR, 122(2), 2017; GRL, 43(26), 2019; *Bossert et al.*, JGR, 122(15), 2017). Stretched domains (e.g., *Fritts et al.*, AGU FM, 2017) can capture the horizontal extents of wave fields, allowing higher resolution where needed. However, numerical strategies that control resolution in all dimensions at high altitudes provide further benefit, dramatically reducing the cost of over-resolved solutions in the diffusive thermosphere. Our approach is to apply adaptive mesh refinement (AMR), albeit with the needs to mitigate transients and to define refinement criteria that still capture nonlinear evolutions.

We report recent progress on the numerics and underlying model physics of the Model for Acoustic-Gravity wave Interactions and Coupling (*Zettergren and Snively*, JGR, 120(9), 2015, and references therein). MAGIC is now implemented in ForestClaw (*Calhoun and Burstedde*, arXiv:1703.03116, 2017), which is an AMR and solver library, using p4est mesh management (*Burstedde et al.*, SIAM JSC, 33(3), 2011), and Clawpack solvers (*Clawpack Development Team*, 2002-2020; *LeVeque*, JCP, 131, 1997). "**MAGIC Forest**" thus includes the full feature set of 2D MAGIC, with its latest numerics, enabling AMR for surface-to-space (0-400+ km) AGW dynamics in large (~1000s km) domains, with calculation of species densities and airglow observables. We also introduce the new *3D* MAGIC Forest in an "extruded mesh" form that leverages 2D AMR in the horizontal directions. We discuss the scalability and performance characteristics of these new models, leveraging AMR to achieve high resolutions only where needed, achieving up to *orders-of-magnitude* speedups. We demonstrate applications in long-range, multi-scale AGW propagation and coupling across deep altitude spans and extensions to the ionosphere.

MAGIC (*Snively and Pasko, 2008; Snively, 2013; Zettergren and Snively, 2015*)

- **Model for Acoustic & Gravity wave Interactions and Coupling**
- Based on finite volume method (FVM) (*LeVeque*, 2002) for **nonlinear**, **compressible**, **Euler** equations, with **Navier-Stokes viscosity and thermal conduction**.
- Solves advection or conservation equations for major and minor species mass fractions, mixing ratios, or number densities.
- Solves Riemann problems in a **flux-difference-splitting (*f-wave*) Roe solver** (e.g., *Bale et al.*, 2002; *LeVeque*, 2002), with "transverse" Riemann solvers for an *unsplit* solution of the Euler equations with gravity.
- Applies **TVD 3rd order (CFL-dependent) flux limiters** (e.g., *Kemm*, 2011, 2012).
- Works/complies with Clawpack (www.clawpack.org) libraries.

+ ForestClaw (*Calhoun and Burstedde, 2017*)

- **Forest-of-Trees Parallel AMR Library for Conservation Laws (Cell-based FVMs)**
- Incorporates Clawpack (*or other*) solvers for conservation laws with source terms, with multi-rate time stepping and multi-block configuration (e.g., *LeVeque*, 2002).
- Enables efficient, scalable domains in generalized geometries with multiple physics.
- Implemented within **p4est** library for AMR mesh management (*Burstedde et al.*, 2011).
- **MAGIC 2D AMR in 2D** (*x-z* or axisymmetric *r-z*) **or 3D** (refining *x-y* in Cartesian *x-y-z*).

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0$$
$$\frac{\partial}{\partial t}(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\mathbf{v} + p\mathbf{I}) = \rho\mathbf{g} + \nabla\cdot\boldsymbol{\tau}$$
$$\frac{\partial E}{\partial t} + \nabla\cdot\{(E+p)\mathbf{v}\} = \rho\mathbf{g}\cdot\mathbf{v} + \underbrace{\boxed{(\nabla\cdot\boldsymbol{\tau})\cdot\mathbf{v}}}_{\text{Approximation}} + \kappa\nabla^2 T$$
$$E = \rho\epsilon + \frac{1}{2}\rho(\mathbf{v}\cdot\mathbf{v})$$
$$\tau_{ij} = \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k}\right)$$

In contrast to atmospheric models designed for forecasting, **MAGIC Forest** is designed for *experiments* conducted in specific environments over short periods of time. E.g., it is used for transient wave evolutions from meteorological processes and manmade or natural hazards, to simulate wave propagation, processes, and effects on observable systems. In traditional MAGIC, approximations are applied for efficiency; see *Zettergren and Snively* (2015). However, the use of AMR in MAGIC Forest enables flexibility, both to resolve target dynamics in large domains and, in 2D *x-z* or, pending, full-3D AMR in *x-y-z*, to ensure that the mesh is appropriately-resolved at high altitudes where viscosity is very high. The use of AMR for scaling allows for a fully-explicit numerical solution across broad and deep domains, solving the hyperbolic and parabolic parts of the problem over single-stages & steps. Thus, AMR unlocks efficiency to enable additional physics with simpler solvers.

In the inviscid limit, note that MAGIC Forest still retains its shock-capturing capabilities (Figure 1), and resolves instability leading to turbulence as an "implicit" large eddy simulation (ILES) for compressible dynamics.

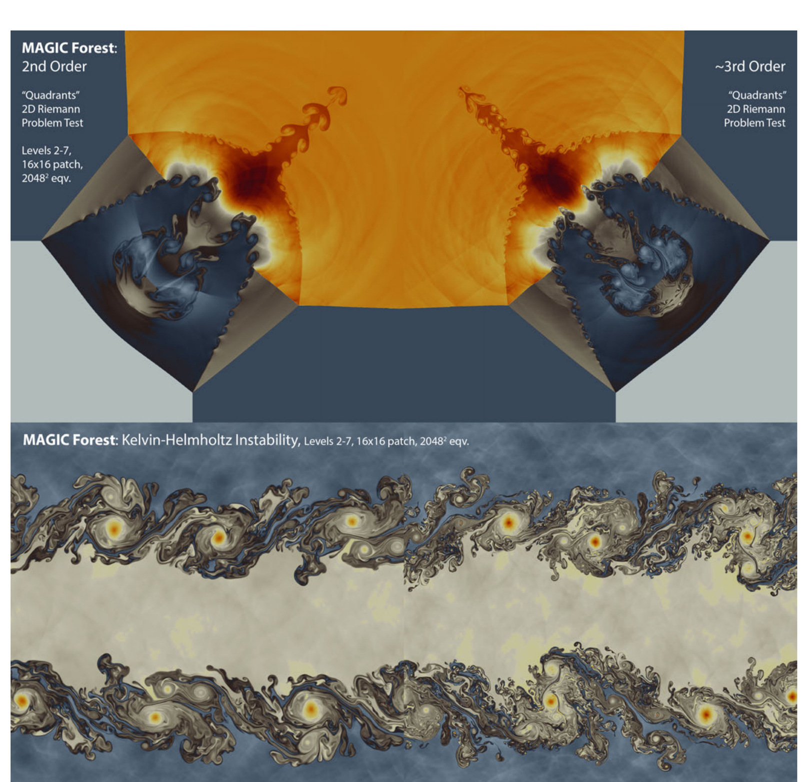
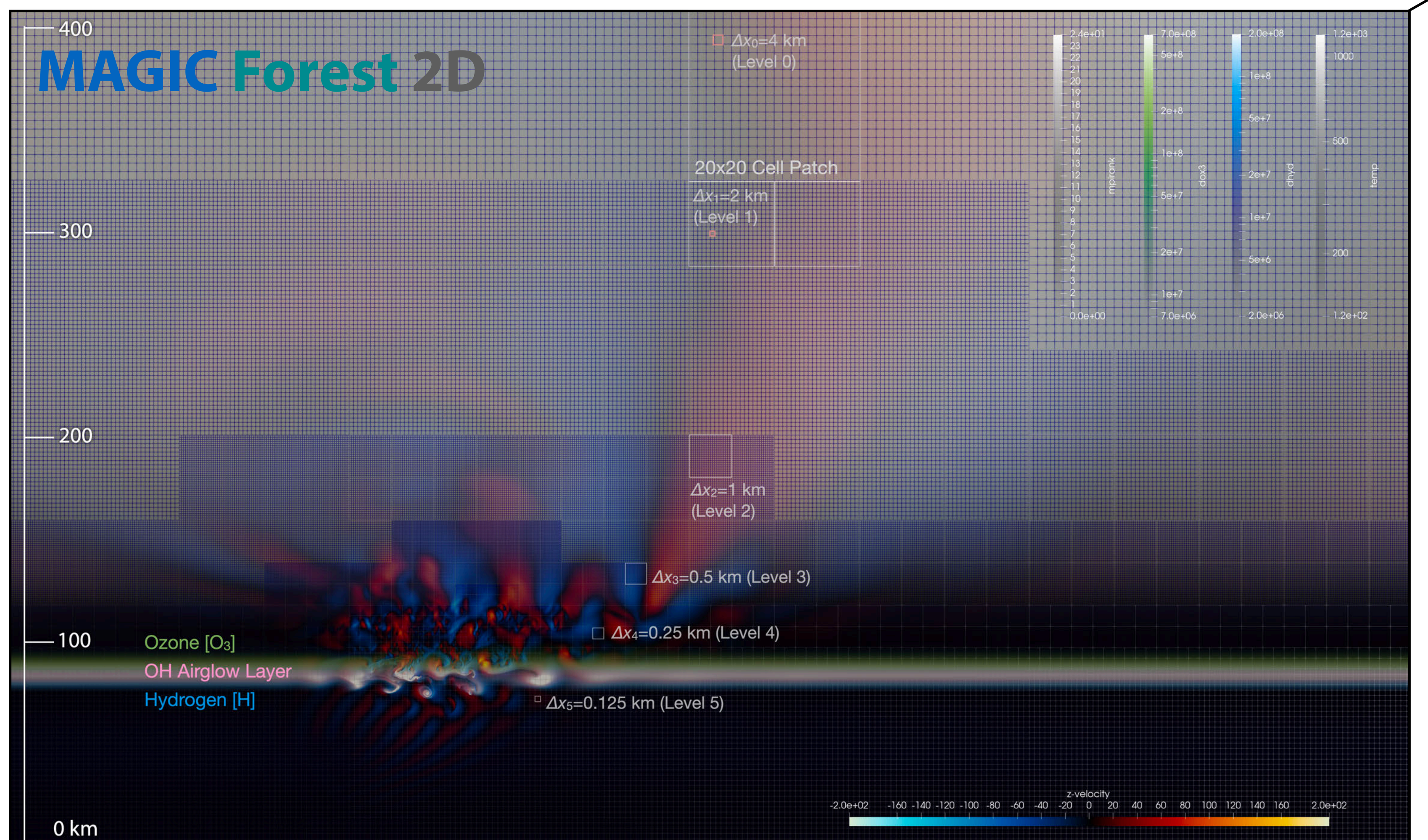
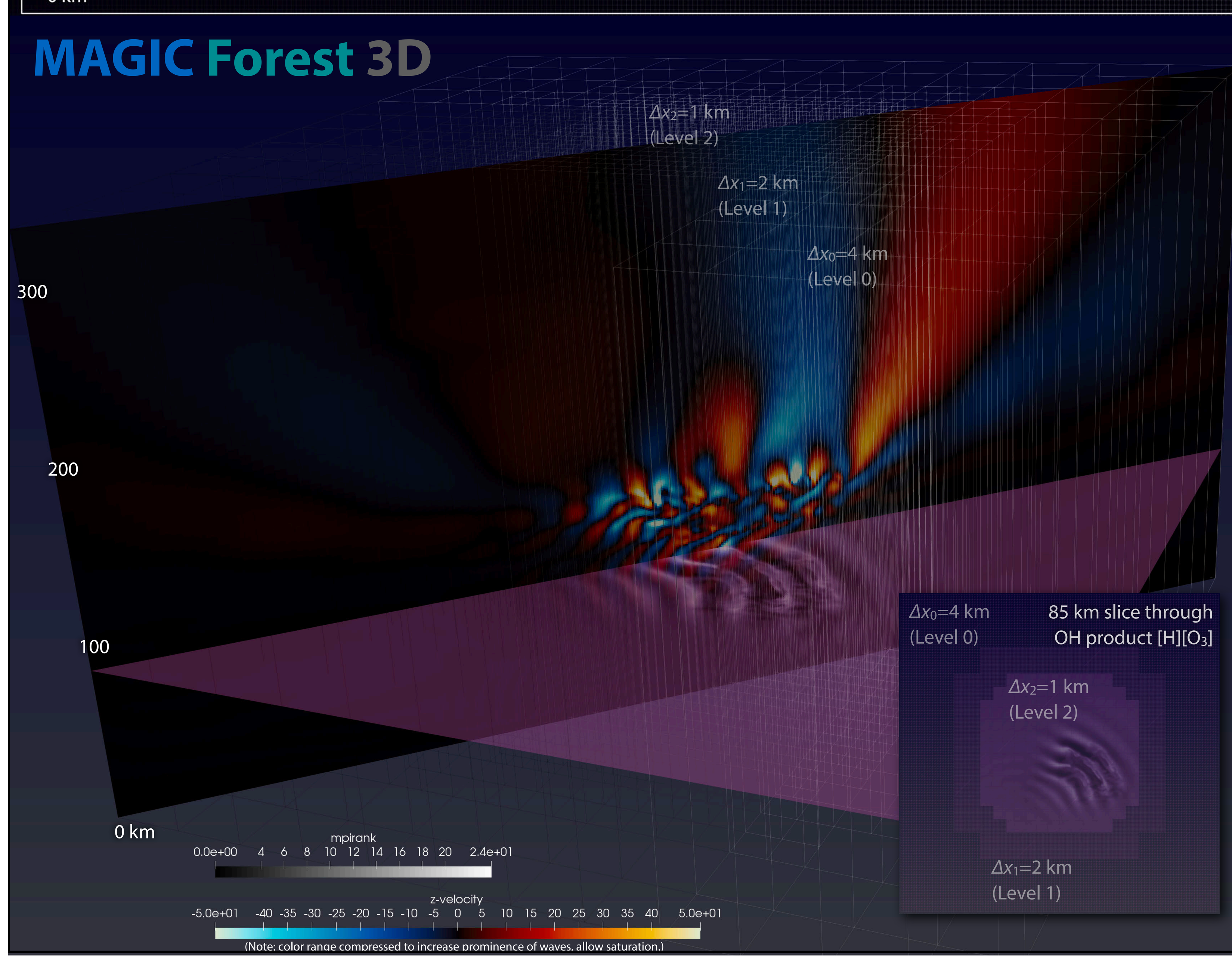


Figure 1: **MAGIC** is based on a robust un-split finite-volume wave-propagation method (e.g., *LeVeque*, 2020; *Kemm*, 2011; *Calhoun and Burstedde*, 2017), and naturally supports inviscid shocks and discontinuous solutions. Shown here are reference code verification tests for 2D Riemann problems and Kelvin-Helmholtz instabilities, comparing (early) 2nd and (current) 3rd order MAGIC Forest formulations.





Major and Minor Species Accounting:

$$\frac{\partial \chi}{\partial t} = -\mathbf{v}\cdot\nabla\chi$$

1. Solve ***advection*** equations for species mass fractions (Figure 2), from which composition is defined, *or* approx. mixing ratios.
2. Define "mass fractions" for the **major gas**: $X_S=\rho_S/\rho$ for s=O or O_2, where $\rho_{N2}=\rho-\rho_O-\rho_{O2}=\rho(1-X_O-X_{O2})$, to eliminates an equation, and optionally evolve equation of state (*Piñeyro*, MS, 2018).
3. Define *approximate* mixing ratios for the **minor species** (e.g., [Tracer]/[O+O_2+N_2]); or, solve with continuity equation with minor penalty and slightly less-robust numerics.
4. Optionally, include **chemistry**, e.g., for OH(v) emissions (*Snively et al.*, https://doi.org/10.1029/2009JA015236, 2010, and references therein), or drive **GEMINI** ionospheric model.
5. *In-Progress*: Species diffusion (in a multi-component gas mixture) by *Piñeyro and Sabatini* (Acs. Soc. Am., 2021), testing for 1D problems; for minor (passive) or major (active) species.

Environments, Sources and Boundary Conditions:

As with prior versions, **MAGIC Forest** is typically driven time-dependently using analytically defined source terms — demos shown here use isolated Gaussian body forces and energy release. MAGIC environments are provided from empirical models (e.g., *Drob et al.*, 2015, *Emmert et al.*, 2020, and references therein) or prepared data from forecasts or measured data. Boundary conditions are consistent with traditional MAGIC, and new/efficient data-driven source routines for mapped volumetric inputs or surface motions (e.g., *Heale et al.*, 2019; *Inchin et al., 2021)* are in development.

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Applications of MAGIC Forest:

- Acoustic-gravity wave (AGW) propagation, evolution, nonlinear/linear dissipation, and secondary waves & effects extending across a wide range of spatial scales (<km to 1000s km).

MAGIC Forest 2D Demo: (*~overnight on 25 (out of 28) cores of Xeon W desktop workstation*)

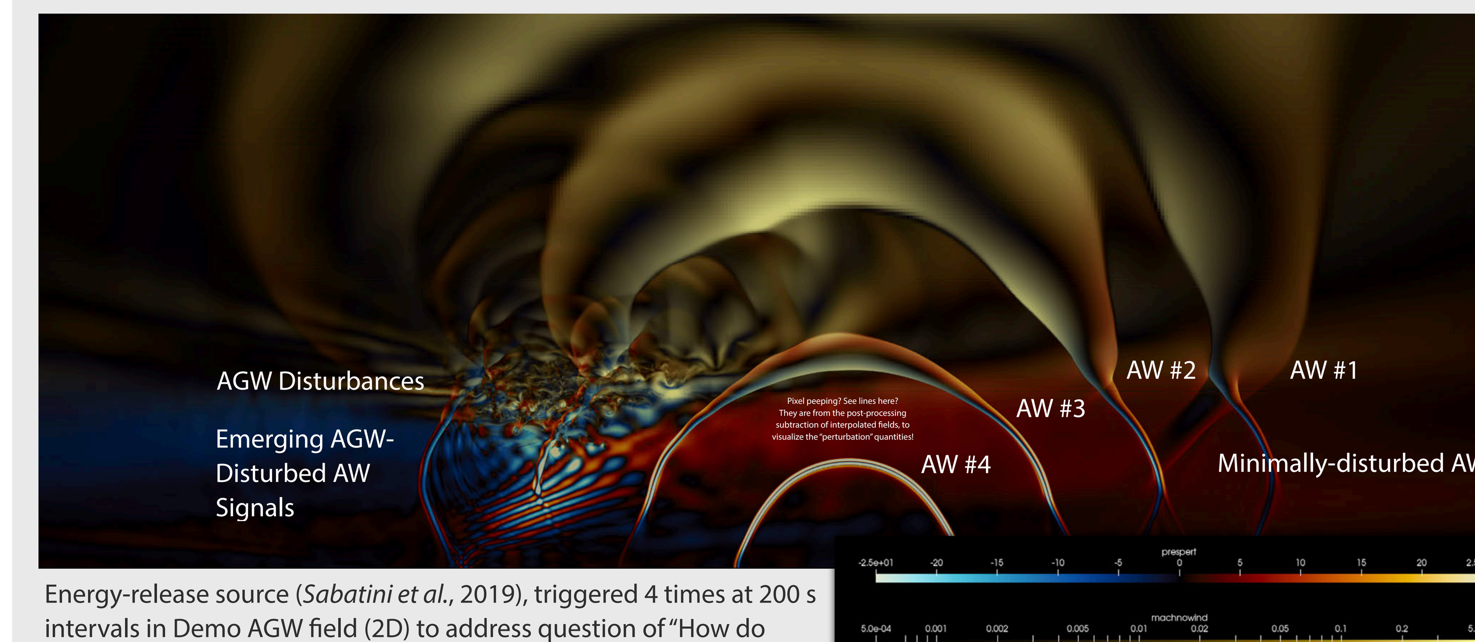
- Part of 1600 x 400 km 2D AMR domain, spanning 20x5 blocks of 20x20 cells at level 0.
- Resolution from 4 km to 125 m (levels 0-5); >240 km default 4 km, <80 km default 125 m.
- Source: ~20 km wavelength in Gaussian envelope, 8.16 min period.
- Inclusion of OH layer [H], [O_3], plus [Na] (see below) and [n_e] tracers, and major species.

Each Frame, +400 seconds — Breaking wave effects on [Na] layer.

MAGIC Forest 3D Demo: (*~2 days on 25 (out of 28) cores of Xeon W desktop workstation*)

- Part of 480 x 480 x 320 km 2D static MR domain, 12x12 blocks of 20x20x320 cells at level 0.
- Horizontal resolution from 4 km to 1 km (levels 0-2); vertical resolution 1 km, static.
- Source: ~22 km wavelength in Gaussian envelope, 45 deg. orientation, 10.47 min period.
- Inclusion of OH layer [H], [O_3], plus [Na] and [n_e] tracers, and major species.

- Acoustic wave (AW) pulse and shock (N-wave) propagation (mHz to ~Hz) from surface to space.
- Propagation of AWs & AGWs of diverse scales that disperse broadly from transient sources.
- **Interactions of AWs and AGWs**, for theory and sensing (*Sabatini and Snively*, S51A-02, 2021):



Energy-release source (*Sabatini et al.*, 2019), triggered 4 times at 200 s intervals in Demo AGW field (2D) to address question of "How do ambient wave fields influence AW signals of natural hazard events?"

Big Picture of MAGIC Forest (and *Trees* GEMINI):

MAGIC is part of a *suite* of models being reformulated for new investigations — targeting higher frequencies, smaller scales, and larger and more-realistic environments — under the DARPA DSO's AtmoSense program's AIRWaveS project (Atmosphere-Ionosphere Responses to Wave Signals), as basic research. MAGIC simulates mechanical wave (AGW) effects on the atmosphere and the ionosphere via coupling to **GEMINI** (Geospace Environment Model for Ion-Neutral Interactions), as well as their signatures that may be remotely-sensed. New **ForestClaw/p4est** implementations of MAGIC and GEMINI will thus also be combined with tools for scalable mappings between models, and integration/analyses of observable quantities for synthetic data comparisons to reality.

Refinement Criteria and Mesh Initialization:

- Uses infrastructure of built-in **ForestClaw** (latest-version) refinement tagging, however…
- … refinement/coarsening must be decided based on quantities that can be scaled by density (e.g., pressure, velocity, derivatives thereof) to enable simple criteria that work across a domain.
- *Practically, we adopt a mix of static and adaptive refinement strategies. (Await our papers please!)*

Figure 2: Specifications of atmospheric composition, shown here from *Piñeyro* (MS, Thesis, ERAU, 2018), as defined in **MAGIC/MAGIC Forest** (e.g., from MSIS). These may be specified statically or evolved time-dependently.

Notes:
MAGIC's Riemann solver supports inviscid shocks between its major species.

Neutral winds, temperatures, and densities are defined from other models, data, or approximations. MAGIC's scheme is well-balanced, so that mean state profiles require minimal preparation.