Untangling deterministic and non-deterministic ocean processes in SWOT observations

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1. Summary

The NASA/CNES Surface Water Ocean Topography (SWOT) mission is a ground-breaking future satellite mission that will, for the first time, provide a global view of the ocean at submesoscales (**Figure 1**). The unique nature of future SWOT observations poses significant practical challenges, however. This project will support the scientific goals of the SWOT mission by addressing two key challenges:

- separating *deterministic processes* (including balanced mesoscales and internal tides) from *intrinsically random processes*, in particular submesoscale currents and unbalanced internal waves,

- temporally interpolating the deterministic component of SWOT observations to produce maps of SSH in space and time while retaining the effect of non-deterministic processes in a statistical sense.

This project aims to address these challenges by developing novel data-driven techniques to untangle deterministic and non-deterministic upper ocean processes from future SWOT observations. By bringing together cutting-edge developments in Lagrangian filtering and stochastic modelling along with detailed *in-situ* observations and high-resolution non-hydrostatic numerical simulations, the results of this project will deepen our understanding of the interaction of submesoscale processes and internal waves and their role in Earth's oceans and climate.

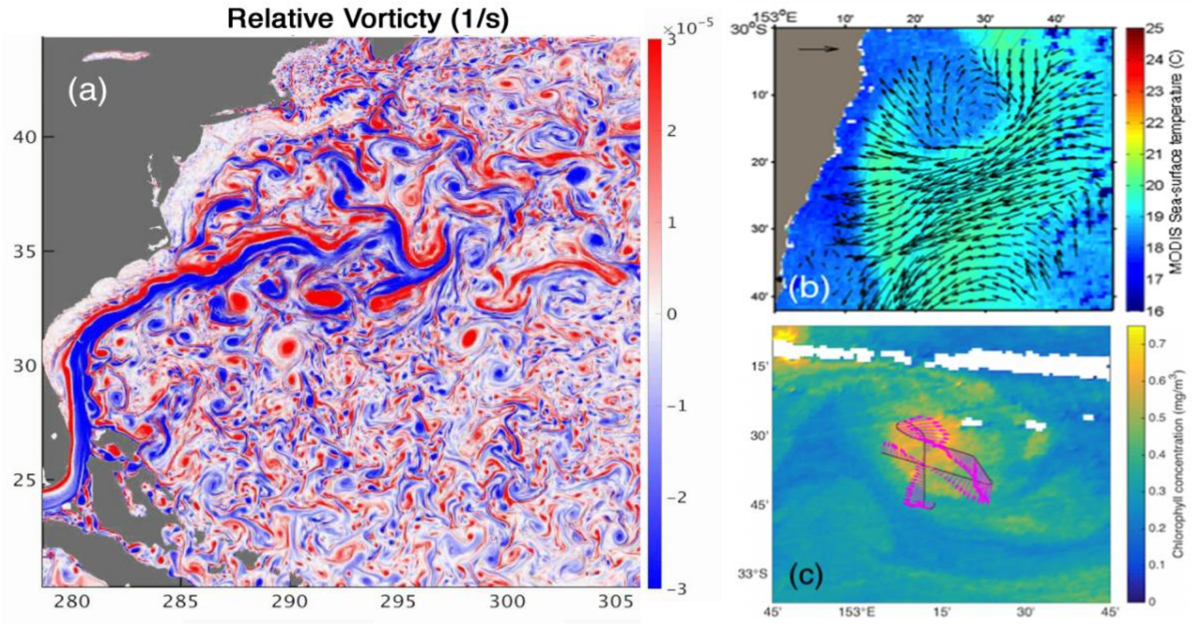

Figure 1. *Submesoscale dynamics in the upper ocean. (a) Surface vorticity in the Gulf Stream from a 1/48° degree global simulation (Su et al. 2018). (b) Submesoscale frontal eddy (~40 km) observed off SE Australia in HF radar and SST imagery. (c) A submesoscale eddy (~15 km) in the Tasman Sea sampled with sea-surface chlorophyll and shipboard ADCP.*

2. Experimental Objectives

SWOT will provide 2D snapshots of sea-surface height (SSH) from mesoscales down to wavelengths of approximately 15 km (Fu and Ubelmann, 2014). However, the time between successive passes will be limited by SWOT's orbit, which will have a 20.86-day repeat cycle with a 10-day subcycle. [There will also be a fast-sampling phase with a 1-day orbit.] An important consequence of the mismatch between spatial and temporal resolutions is that rapidly evolving small-scale unbalanced motions will be undersampled in time and can become entangled with the more slowly evolving balanced dynamics (Qiu et al. 2017; 2018).

The aim of this project is to develop and validate new methods for untangling deterministic and non-deterministic dynamics from future SWOT observations. In this context, deterministic means simply that the correlation timescale is comparable or longer than the sampling time. Thus, deterministic dynamics remain temporally coherent from one observation to the next. At SWOT spatial resolutions, mesoscale dynamics, evolving on timescales of weeks to months, are generally deterministic. Likewise, barotropic tides are highly predictable in numerical models and satellite observations.

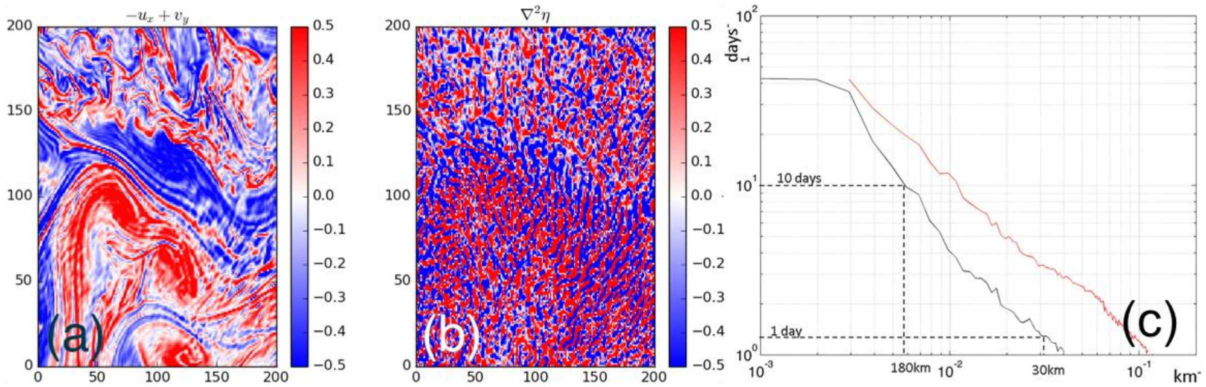

Figure 2. *(a) Surface relative vorticity in a 4°x4° region of the Gulf Stream from a 1/48° global ocean simulation. (b) Simulated SWOT observations of the same flow. The signal is dominated by internal waves. Credit: J. Wang and D. Menemenlis, NASA JPL. (c) Decorrelation time vs wavelength, calculated from MITgcm model of the North Atlantic. Adapted from Morrow et al. (2019).*

Ocean processes that evolve and decorrelate on timescales much faster than the sampling time are effectively random and unpredictable. For the SWOT mission, this includes submesoscale processes, which evolve on timescales of days (McWilliams 2016), and unbalanced internal tides and other internal gravity waves, with periods of minutes to hours. SSH variations due to internal waves are a particular challenge for SWOT observations because their spatial scales overlap with those of balanced motions at submesoscales and so can dominate the SSH signal and derived quantities such as geostrophic velocities and surface vorticity (Qiu et al. 2017; 2018; **Figure 2**).

Note that the distinction between deterministic and non-deterministic motions is separate from (though related to) the distinction between balanced and unbalanced motions. Baroclinic internal tides are unbalanced (they have frequencies greater than the Coriolis frequency) but can remain correlated over long timescales and so, in principle, are predictable (for a review of recent progress, see, e.g. Arbic et al. 2018). In contrast, submesoscale currents evolve rapidly (on timescales of hours to days) but have both balanced and unbalanced flow components (McWilliams 2016). Put another way, the balanced/unbalanced separation is a property of the ocean dynamics, whereas the deterministic/non-deterministic separation is a property of the observing system.

Our project seeks to address these knowledge gaps by answering three core research questions:

1. How "predictable" are upper ocean dynamics at SWOT scales?

2. How can we effectively separate nondeterministic and deterministic dynamics in SWOT observations?

3. How can we smoothly interpolate deterministic dynamics between successive SWOT observations?

3. Approach

3.1 In-situ ocean observations

Northwest Shelf (NWS) study site: The Australian Northwest Shelf is located off NW Australia in the Indian Ocean (**Figure 3b**). The region, which has high economic and biological importance, is characterised by a ubiquitous and energetic internal tide due to large-amplitude tidal forcing generated at the continental shelf break. There is also a significant non-stationary internal tide due to seasonal thermocline variability and internal tides generated by the Indonesian Archipelago propagating across the Indo-Australian Basin and interacting with the seasonal Indonesian Throughflow.

The region is also characterised by the presence of large-amplitude mode-1 and mode-2 nonlinear internal waves. Mode-2 internal waves are of particular interest because they can enhance local dissipation, vertical mixing, and horizontal tracer transport in the pycnocline. Submesoscale variability occurs throughout the Indo-Australian Basin particularly in regions where ocean density fronts collide (e.g., during austral Winter when cool shelf water collides with warm ITF water) and in the wake of tropical storms that mainly occur during the austral summer. There is a distinct lack of a strong mean flow exceeding 50 cm/s along the NWS, making the site an ideal location to investigate the interaction of internal tides and submesoscale SSH signals.

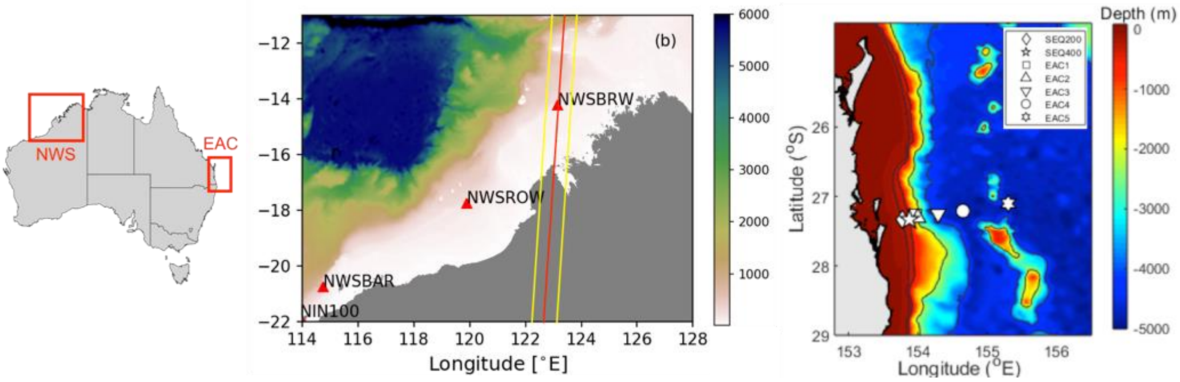

Figure 3. (Left) Study sites for in situ observations and SUNTANS numerical simulations. (Middle) The Northwest shelf (NWS) study site in the Indo-Australian Basin with ongoing IMOS mooring locations indicated by red triangles. The NWSBRW mooring lies under the SWOT 1-day fast-sampling orbit, indicated by the red and yellow lines. (Right) The East Australian Current (EAC) study site in the Tasman Sea. The white symbols indicate ongoing IMOS shelf and deep water moorings.

Australia's Integrated Marine Observing System (IMOS; www.imos.org.au) has carried out sustained observations of the NWS for over a decade, including moorings, glider measurements, and high-frequency radar. This project will focus on the Browse Basin region under the ground track of SWOT's fast sampling orbit. In August 2019, IMOS deployed a through-water-column mooring (NWSBRW; 200m water) under the SWOT 1-day ground track (Figure 3b), consisting of an acoustic Doppler current profiler and a vertical array of temperature and salinity measurements. Observations will continue indefinitely (through the fast-sampling and science phases), with service scheduled every 6 months.

East Australian Current (EAC) study site: The EAC is the western boundary current of the South Pacific subtropical gyre (**Figure 3c**). It dominates the ocean circulation of the Tasman Sea and is highly variable in time due to meandering of the main jet and abundant mesoscale eddies above and below the separation point. Submesoscale flow in the region is characterised by instability of the meandering EAC and generation of frontal eddies with O(1) Rossby number and upwelling associated with elevated chlorophyll-a concentrations.

IMOS has invested extensively in continuous observations and numerical modeling in this region due to its importance to regional climate variability and economic activity in the populous Southeastern Australian coast. These include eight permanent moorings on the continental shelf, two high-frequency (HF) radar systems, and over 30 repeat glider missions, as well as a state-of-the-art ocean ROMS/4DVAR ocean reanalysis that assimilates all available observations in a submesoscale permitting ocean model of the region.

3.2 Numerical ocean simulations

Non-hydrostatic modelling: Algorithms will be tested using modelled ocean datasets generated with the Stanford Unstructured Non-hydrostatic Terrain-following Adaptive Navier-Stokes solver (SUNTANS). For the NWS study site, a domain has previously been set up for the Indo-Australian Basin region and run for 12-months (July 2013 - July 2014) with realistic ocean and atmosphere initial and forcing conditions. The unstructured grid allows both efficient modelling of large regions and focussed studies on smaller regions of interest, such as small islands, where topographically generated internal waves interact with the background flow. Historical IMOS mooring observations collected on the NWS were used for validation. As part of this project, a similar model configuration will be developed for the EAC study site around the EAC mooring array.

In this project, a SUNTANS hindcast will be run for part of the SWOT mission time period and validated using the new observations described above. A similar model grid will be used with further refinements near the observation sites. Grid refinements down to approximately 100 m are necessary to resolve non-hydrostatic processes such as nonlinear internal waves. Furthermore, careful attention will be paid to topographic features like islands, banks and reefs that are important generators of internal waves and eddies yet are unresolved in global scale models.

SWOT simulator: We will perform Observing System Simulations Experiments (OSSEs) of the NWS and EAC study sites using the "SWOT simulator" developed by Gaultier et al. (2016). This tool reproduces the SWOT sampling pattern, measurement error, and instrument noise to simulate synthetic observations of sea-surface height from numerical model output in both global and regional configurations. The simulator first interpolates model output along the SWOT ground track with a 21-day repeat cycle (the science orbit) or a 1-day repeat cycle (the fast-sampling orbit) over a 120 km wide swath with a grid-size of 2 km. The software then generates random instrument noise and geophysical errors estimated from the mission error budget.

3.3 Data analysis

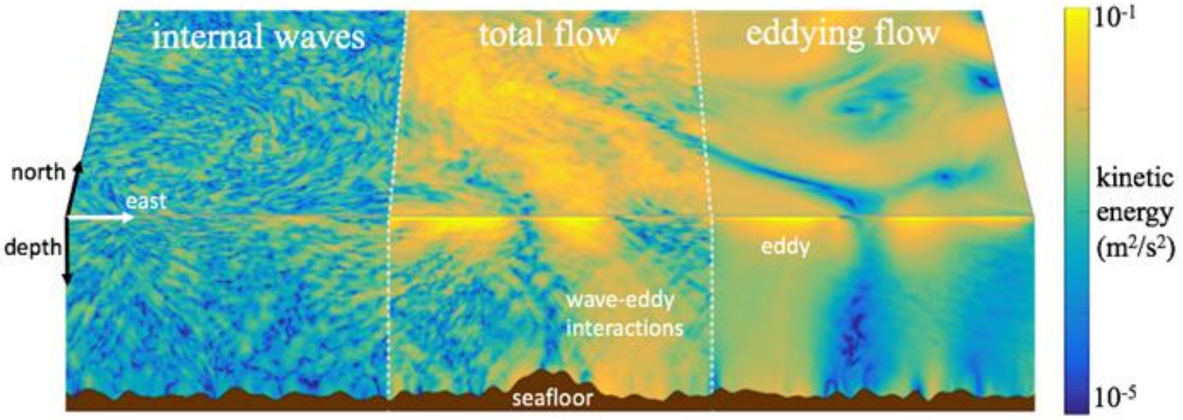

Figure 4. *Example of the Lagrangian filtering method applied to separate waves and eddying flow in high resolution simulations (adapted from Shakespeare and Hogg, 2019). The total kinetic energy (centre) has been decomposed into wave (left) and larger scale eddying flow (right) components.*

Lagrangian filtering: Lagrangian filtering is a novel method for separating the internal wave signal from a complex eddying flow (**Figure 4**). The technique is uniquely suited for application to flow regimes such as the ocean submesoscale where the temporal and spatial scales of eddies and waves overlap, and thus traditional filtering approaches fail (Shakespeare and Hogg 2017; 2018; 2019). The Lagrangian filtering methodology is based on the fundamental physics of internal waves: that an internal wave has a fixed minimum frequency in a flow-following (also called a “Lagrangian”) frame of reference. Any motion in the Lagrangian frame that is less than this frequency may be identified as not being associated with internal waves (or non-wave).

Stochastic data assimilation: In the stochastic data assimilation methodology, a linear stochastic differential equation is used to forecast each complex-valued Fourier amplitude of a dynamical variable such as sea-surface height *h.* This is the simplest parameterization of the interaction of an eddy with a background turbulent flow, and offers two key advantages over traditional DA schemes: (1) it is extremely cheap to implement compared with an eddy-resolving ocean model; and (2) the resulting Bayesian inverse problem can be solved *exactly* using the well-known Kalman filter, which provides the optimal (in a least-squares sense) filtered estimate when the underlying dynamics are linear and the observational and system noise are mean-zero Gaussian random variables. The stochastic filtering approach has been successfully validated using synthetic observations of sea-surface height (Keating et al. 2012) and sea-surface temperature (Keating & Smith, 2015) in idealized ocean models with realistic stratification. We will extend these concepts to synthetic SWOT observations at the two study sites.

Wave-turbulence decomposition: At submesoscales, the SSH signal incorporates geostrophic dynamics, internal waves and tides, and spatially incoherent turbulence, which evolve on different timescales. In the stochastic data assimilation approach, the geostrophic component evolves slowly according to a deterministic model while the fast-evolving internal waves/tides and incoherent turbulence are modelled using a stochastic forecast model: the internal wave/tide signal is modelled using tidal harmonics plus a stochastic component, while the incoherent turbulence is modelled using a Gaussian random noise with prescribed energy spectrum and turbulent decorrelation time-scale.

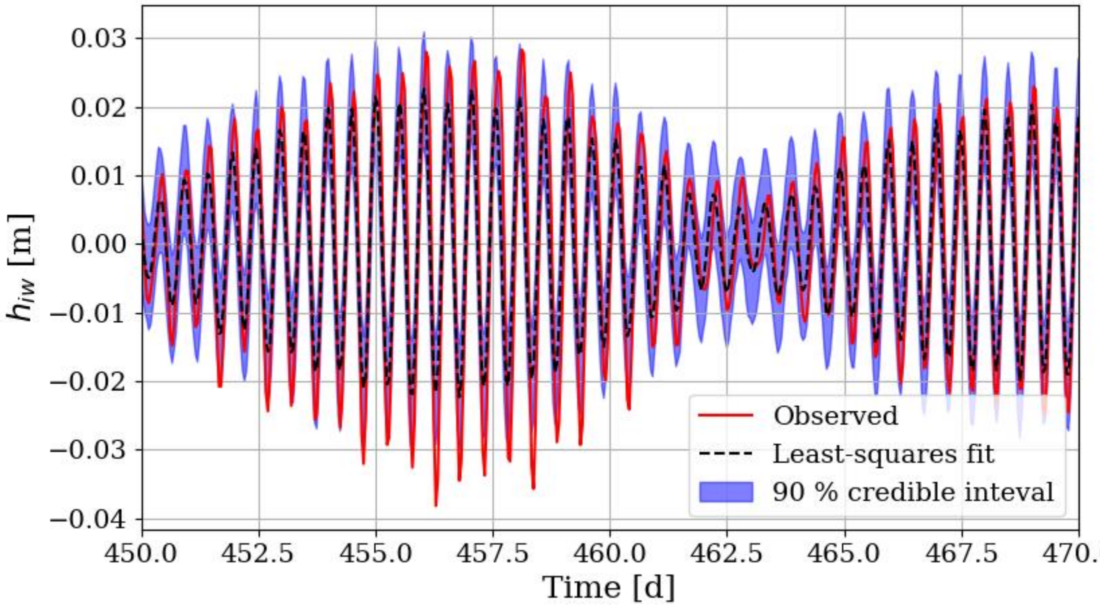

Figure 5*. Sea surface height displacement due to internal tides derived from an in situ mooring (red). Harmonic prediction using least-squares fitting to 5 tidal constituents (black). The blue shaded region indicates the 90 percent credible interval of the posterior distribution (meaning that there is a 90% probability that an observation will fall within these bounds) for the harmonic plus Gaussian noise model derived using a Bayesian parameter estimation technique.*

The internal wave component will be further decomposed into a phase-locked internal tide (coherent, stationary) component and a residual (incoherent, non-stationary internal tide and non-deterministic internal waves). Tidal harmonics for the coherent internal tide will be found via fitting harmonic amplitude to long-time series mooring observations, similar to the way that barotropic tides are removed from current altimetry data. The incoherent internal tide is partly due to phase modulation of the internal tides by variable stratification and mean flow causing frequency smearing. We will estimate the internal wave/tide SSH component using tidal harmonics plus Gaussian noise drawn from an energy spectrum derived from the Lagrangian filtered signal. Typically, least-squares fitting is used to estimate harmonic amplitude parameters. We will use Bayesian inference to estimate the harmonic and noise parameters, and thus obtain a direct measure of uncertainty in the harmonic parameters and the strength of the noise due to the incoherent internal tides and internal waves (**Figure 5**).

Dynamic interpolation of SWOT observations: Ubelmann et al. (2015) proposed a novel method for "dynamic interpolation" of SWOT observations, in which the observed SSH is used as the initial (or final) condition for a quasi-geostrophic (QG) model. Using this model, the sea-surface height is interpolated forward (or backward) in time, significantly reducing interpolation error compared with standard linear interpolation. The method has been implemented with simulated satellite observations in the Gulf Stream and the Mediterranean.

We will extend this promising approach using the stochastic modelling framework to include coupling between slow geostrophic dynamics and fast internal waves, irreversible mixing, and vertical structure, all of which are neglected in the QG model above. We have carried out a pilot study of this stochastic dynamical interpolation scheme and found that inclusion of small-scale forcing representing non-deterministic submesoscale dynamics improves the forecast of mesoscale dynamics due to up-scale interactions (Keating and Rogé, in preparation; **Figure 6**).

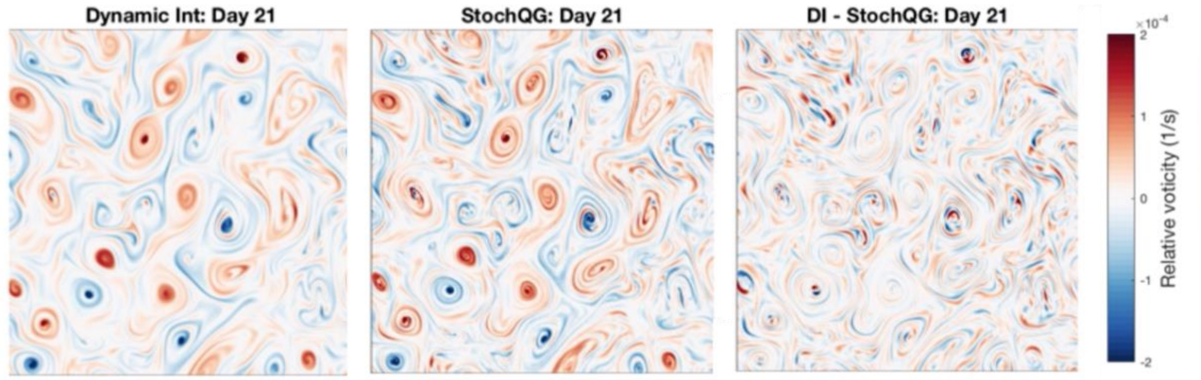

Figure 6. *Stochastic dynamical interpolation scheme applied to spectral QG model output for a submesoscale-rich region of the North Atlantic (the Latmix study site) forced by ECCO hydrography. The snapshots shown are 250 x 250 km sub-regions of a 1300 x 1300 simulation with 43 vertical layers. (Left) The relative vorticity estimated using dynamical interpolation (1-layer QG model) of Ubelmann et al. (2015) after an integration time of 21 days. (Middle) The same field estimated using a stochastic dynamical interpolation scheme in which submesoscale dynamics are represented as a random forcing of the mesoscale field. (Right) The difference between the first two panels. Small-scale forcing in the stochastic dynamical interpolation scheme leads to changes in the mesoscale eddy field due to up-scale interactions. Adapted from Keating and Rogé (in preparation).*

4. Project schedule and Milestones

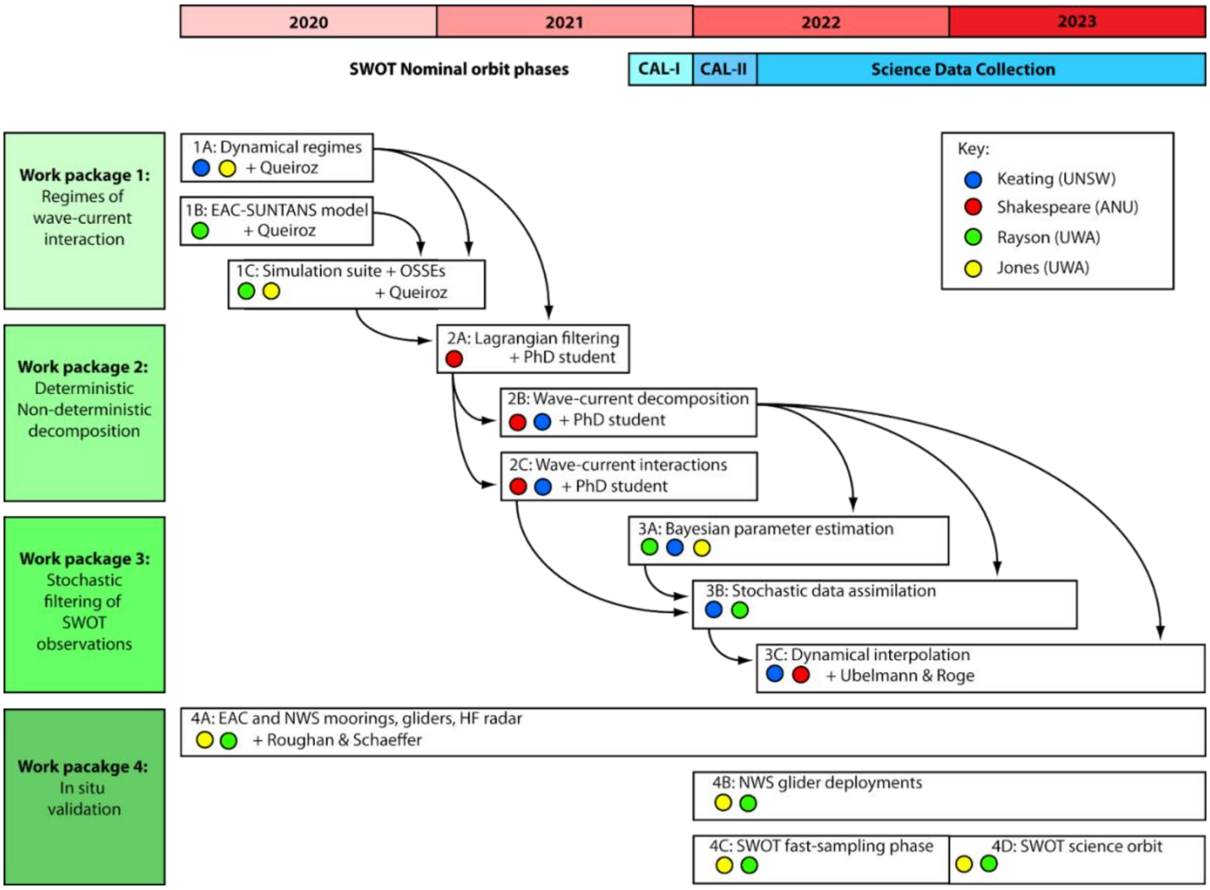

Figure 7. *Milestones, timeline, task flow, and dependencies for the proposed project. Contributions from members of the research team are shown in coloured circles; unfunded collaborators are indicated in the text. The SWOT nominal orbit phases are shown in blue (CAL-I: checkout and commissioning phase, CAL-II: calibration and validation phase, Science Data Collection: science orbit phase). The project timeline will be adjusted if there is a change in the SWOT mission schedule.*

5. References

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