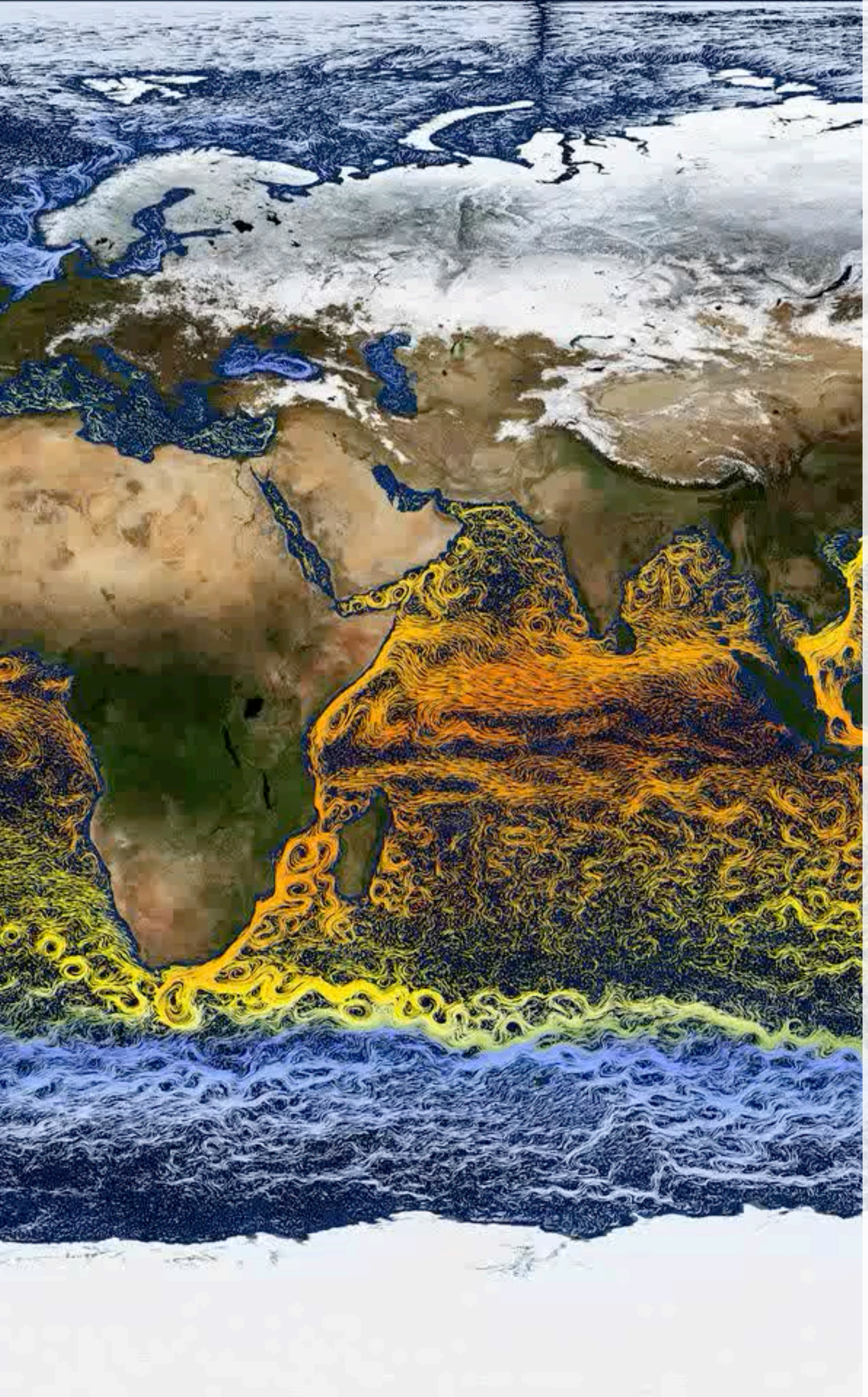


A Particle-in-Cell wave model for efficient wave-ice interaction in CESM

Particle-in-Cell for Efficient Swell - PiCLES

Momme Hell

Woods Hole Oceanographic Institution

Baylor Fox-Kemper, and Bertrand Chapron, Chris Horvat

+ *many others*

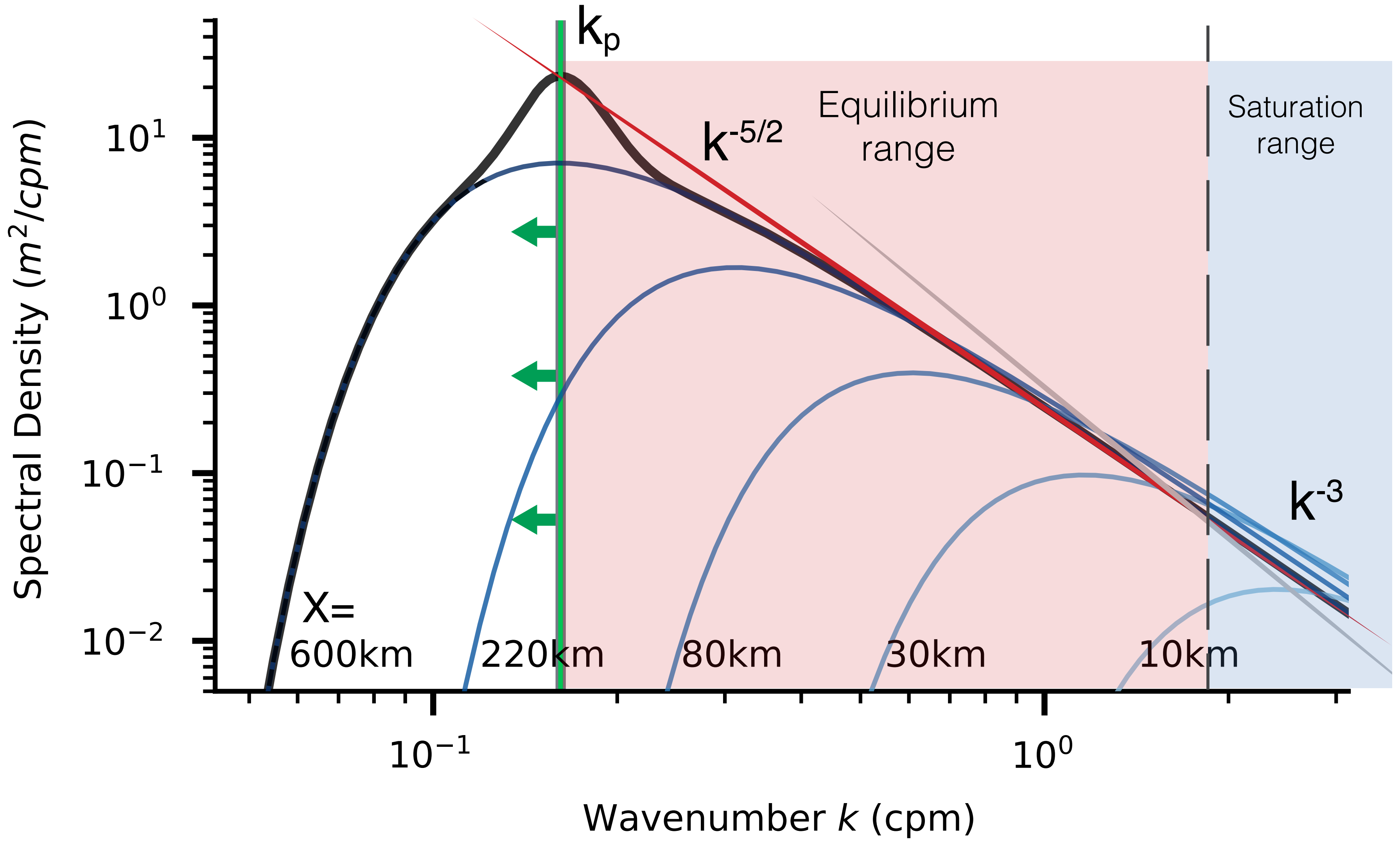
ICERM, Providence 2025

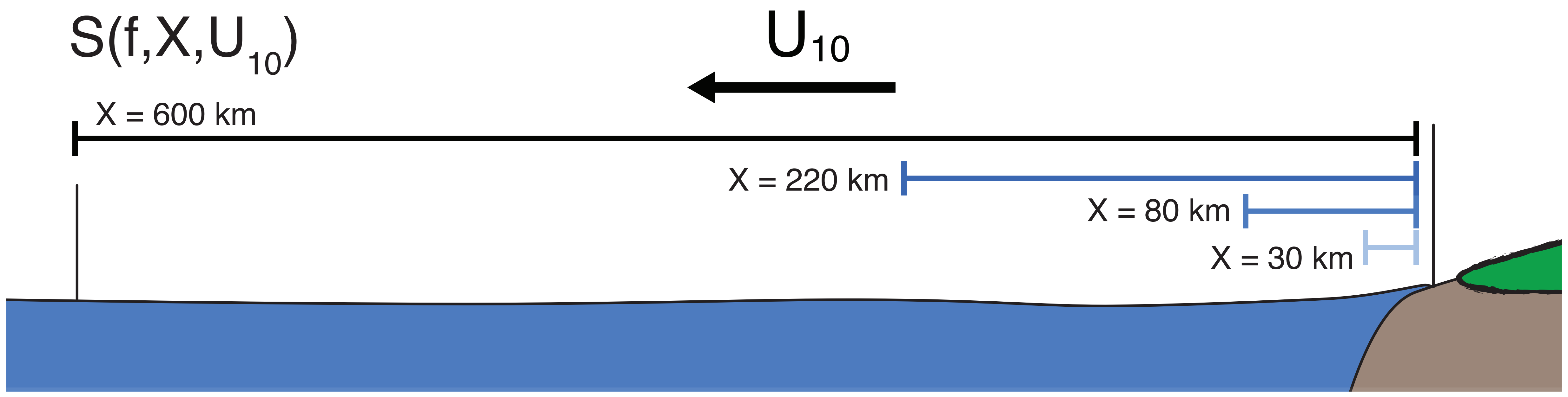
Fetch “laws” for parametric ocean wave spectra

Stationary wave growth and energy transfer in a parametric wave model

(Kitaigorodskii, 1962, Hasselmann et. al 1976)

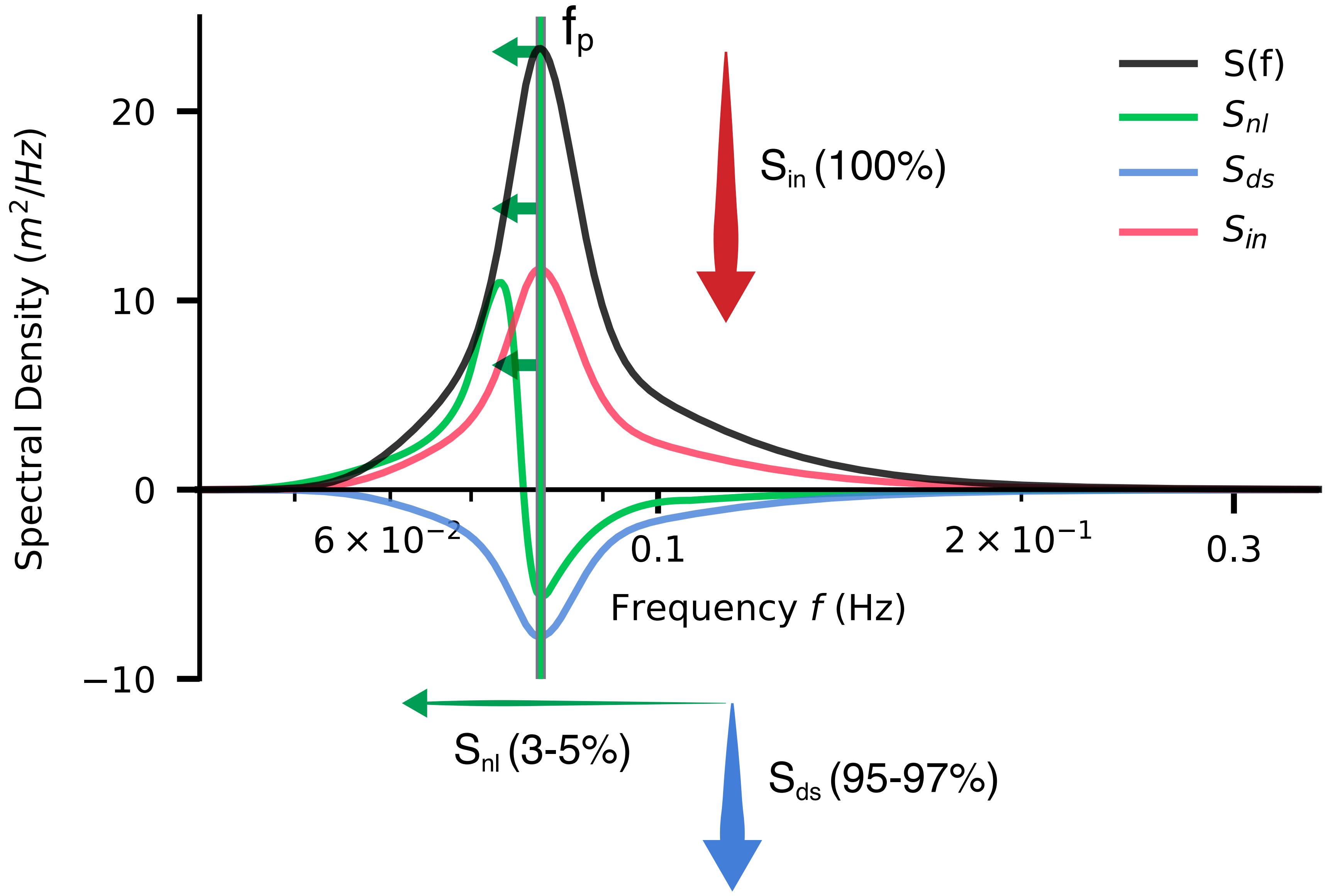
JONSWAP Wave Growth





The frequency spectrum S(f) is modeled as a parametric function depending on **wind speed** (**U_{10}**) over a given **fetch** (**X**).

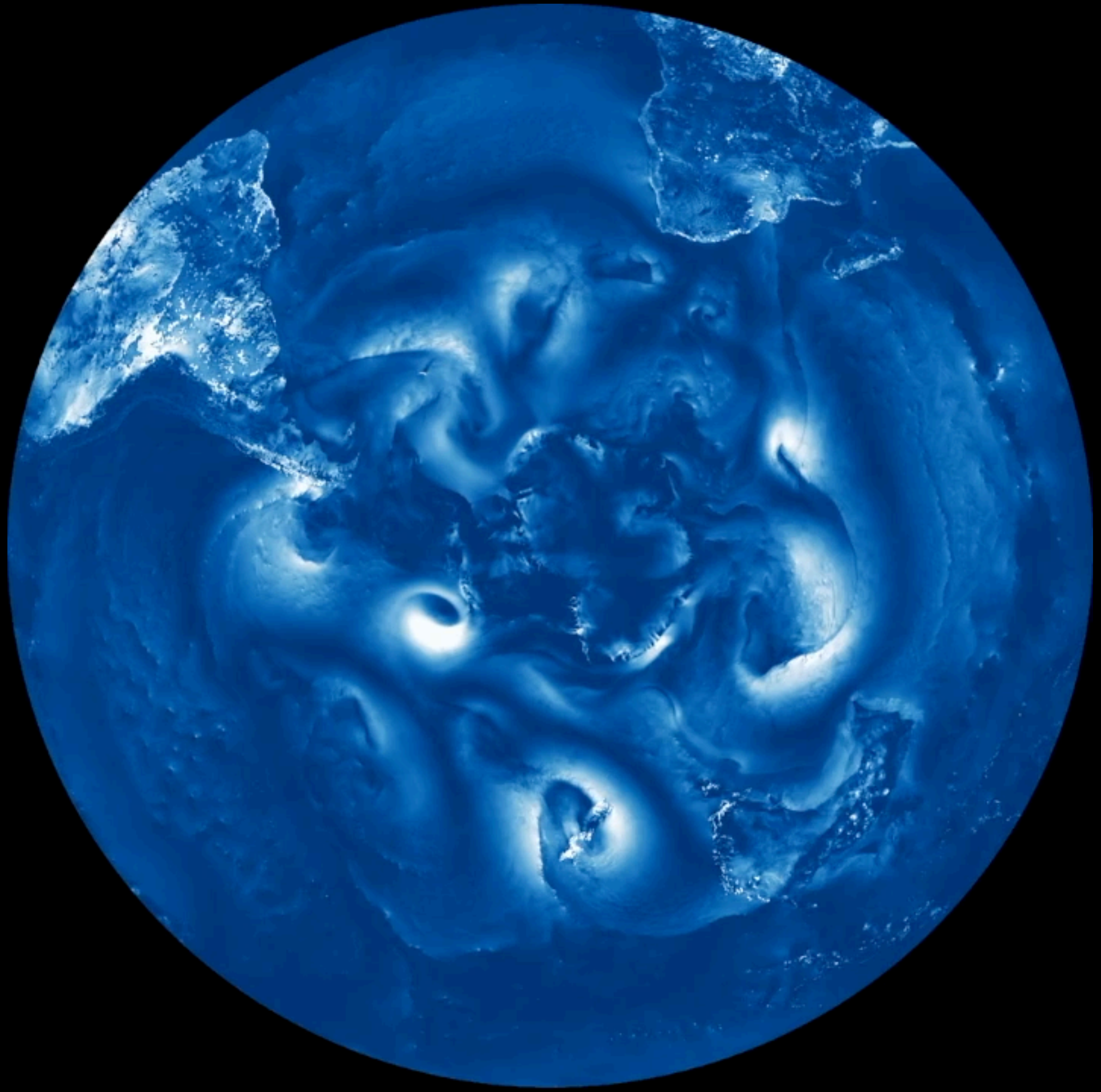
Parametric JONSWAP Model



Spectral growth happens though the dynamic balance in the equilibrium range between
wind input **S_{in}**,
local dissipation **S_{ds}**, and
spectral transfer **S_{nl}**
(Phillips 1985)

Winds and waves are nearly never in equilibrium

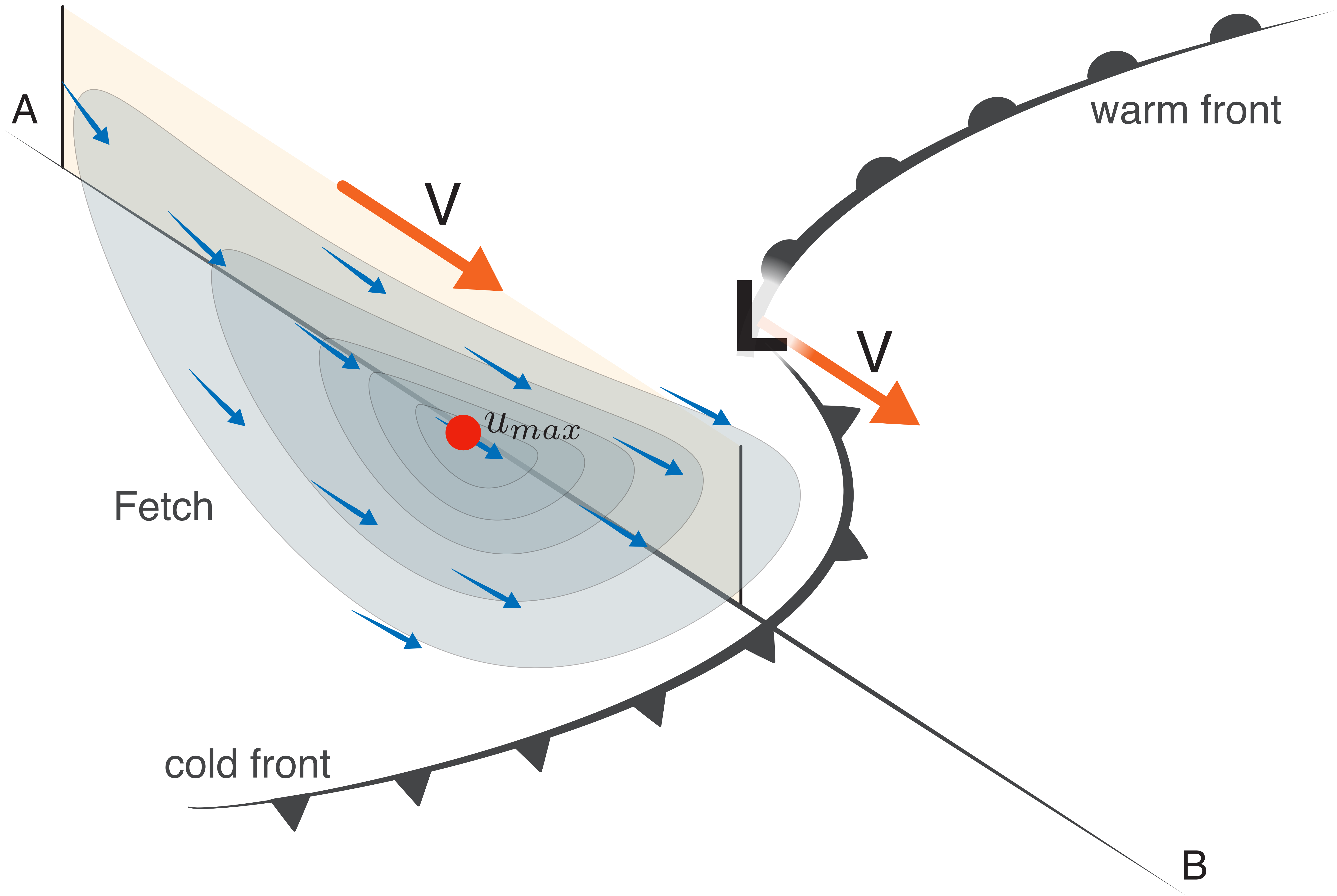
Surface stress
in coupled model



Total surface stress in
NASA/JPL c1440 llc2160 coupled simulation
resolution: Atmosphere - 7 km, Ocean 2-5 km

Let's ride an extra-tropical storm …

… imagine you travel with the storm at its **translational velocity V** and observe the surface wave field …

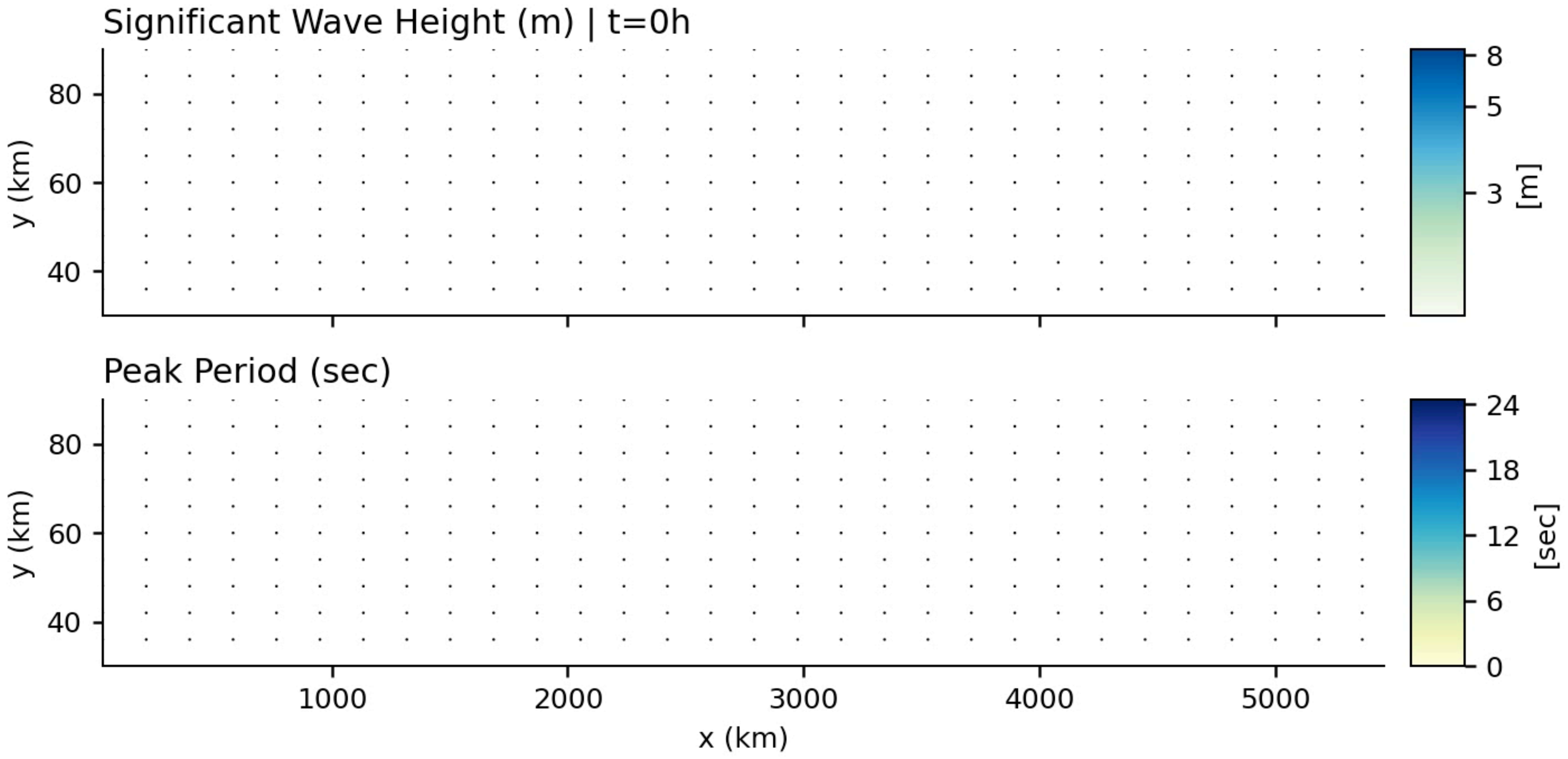


Idealized models of Swell generation under extra-tropical Storms

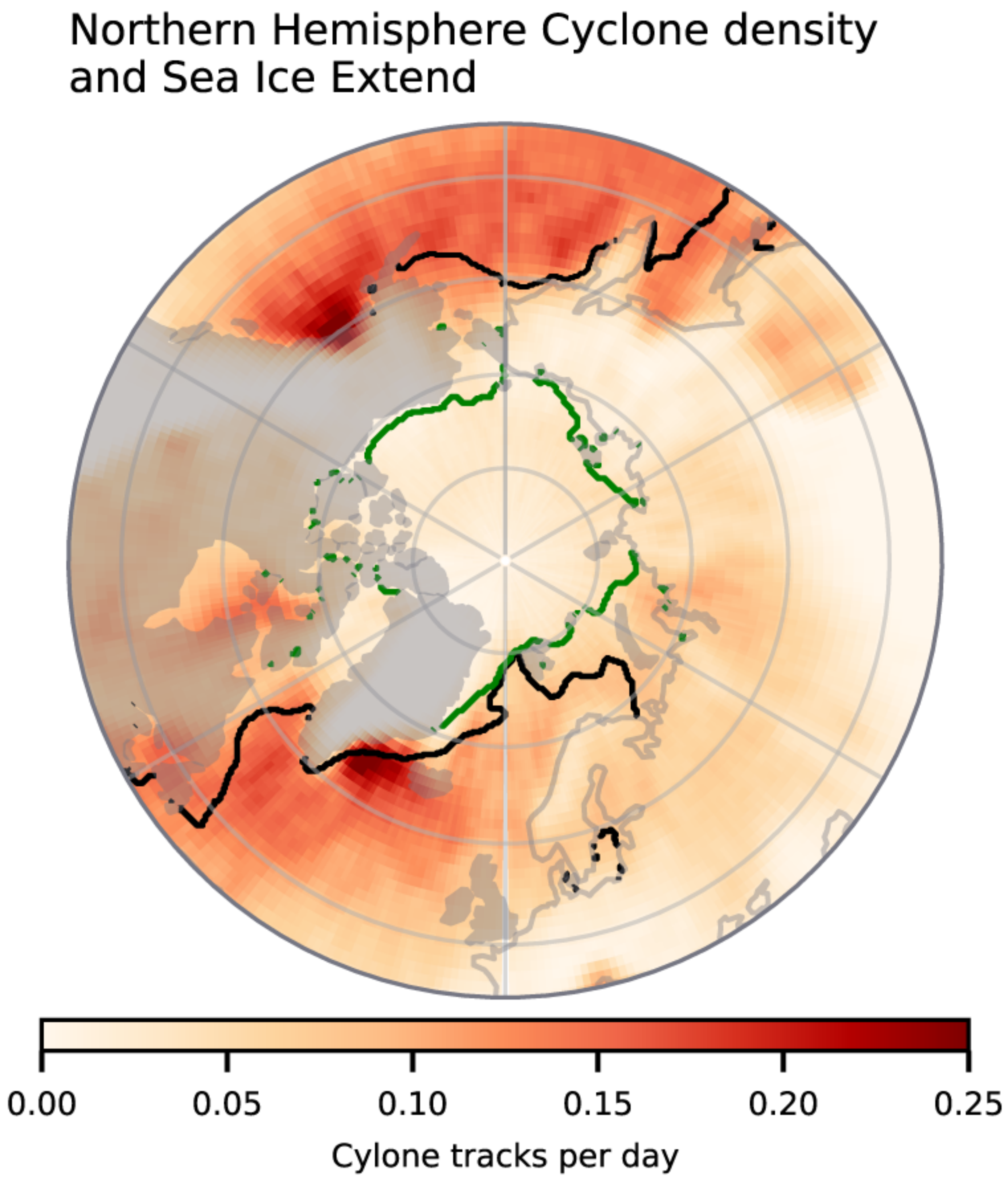
Hell et al 2021, JRG Oceans

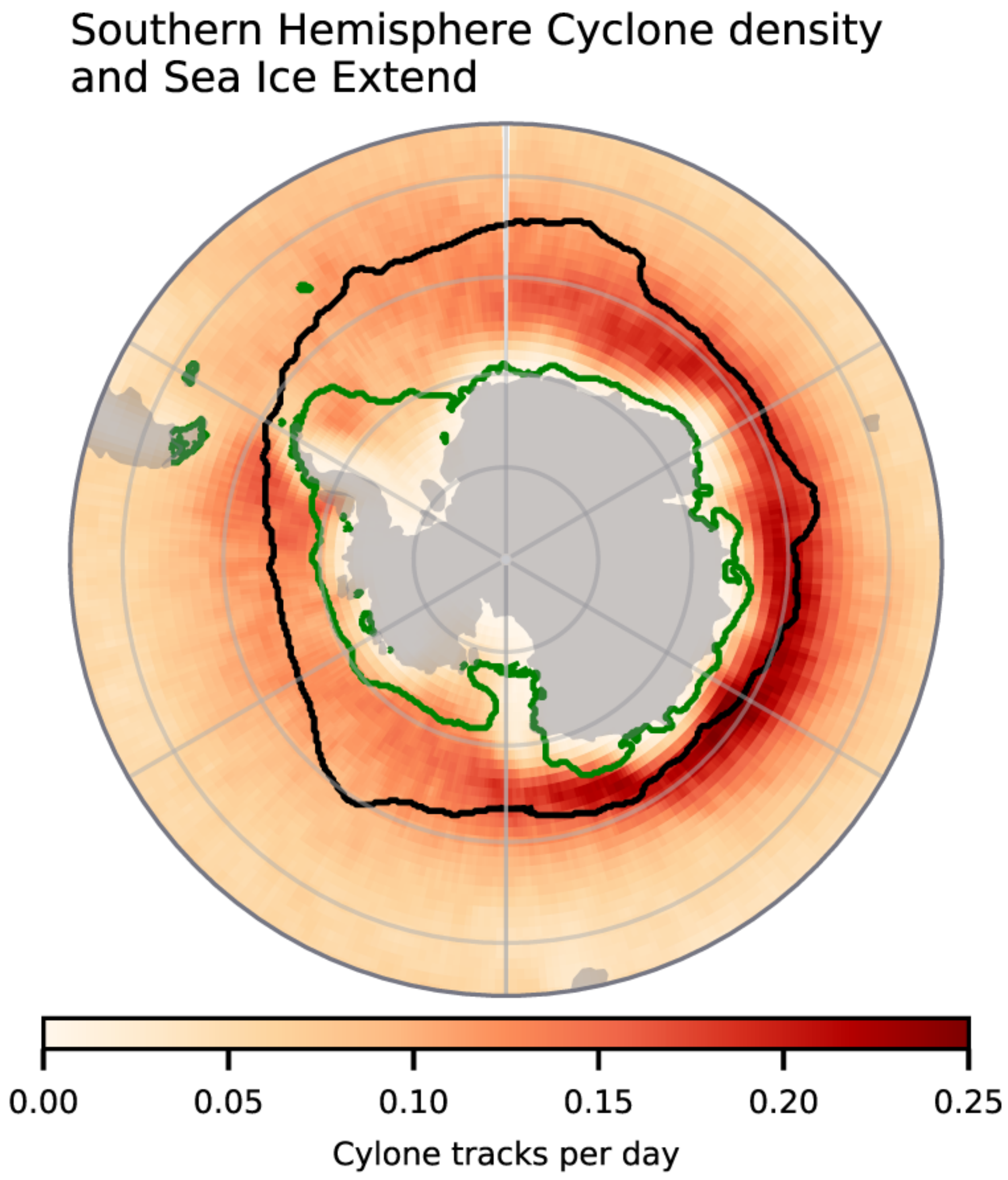
Idealized WaveWatch3 simulation of a moving wind patch

The observer travels with the red dot



Adding Sea Ice: Storms co-locate with the Sea Ice Edge





The storm track density is the largest close to the winter sea ice edge

shading: storm track density (cycles per day)

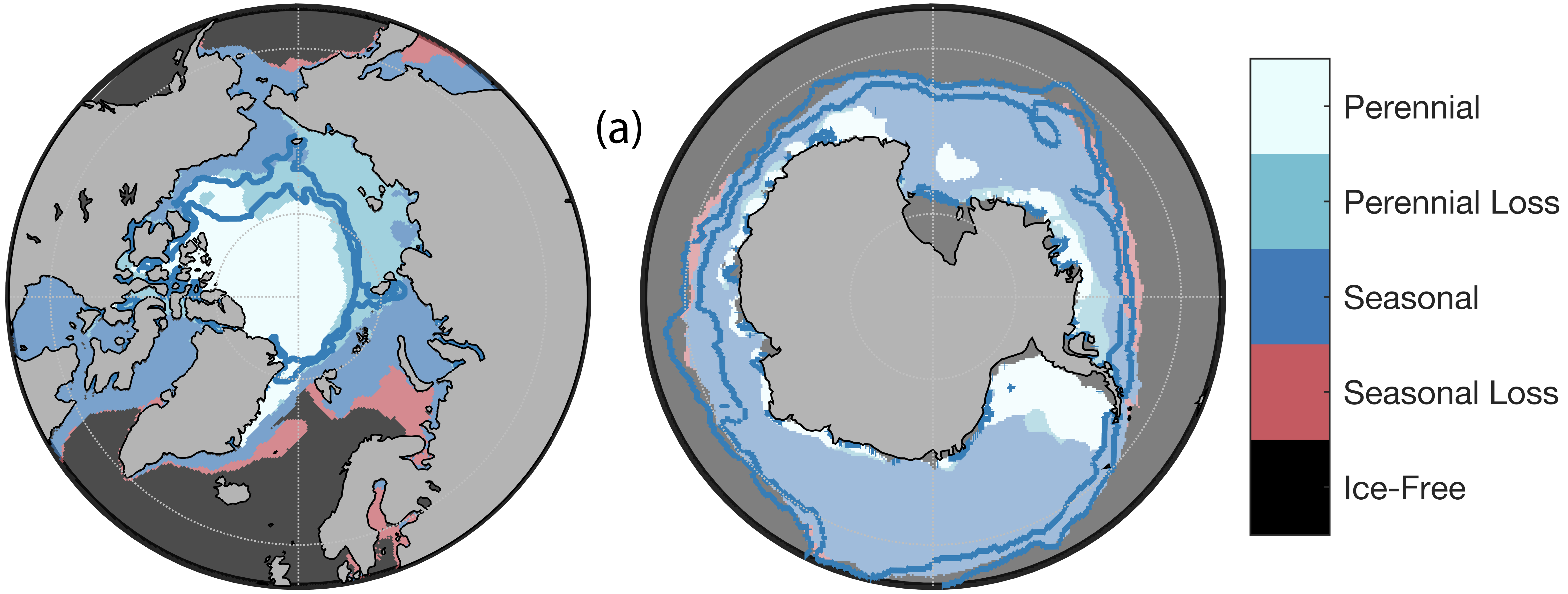
Black lines: Winter maximum sea ice extend

Green lines: Summer minimum sea ice extend

In the **Southern Ocean, large wind-sea and swell variability** govern wave-ice interaction and the MIZ

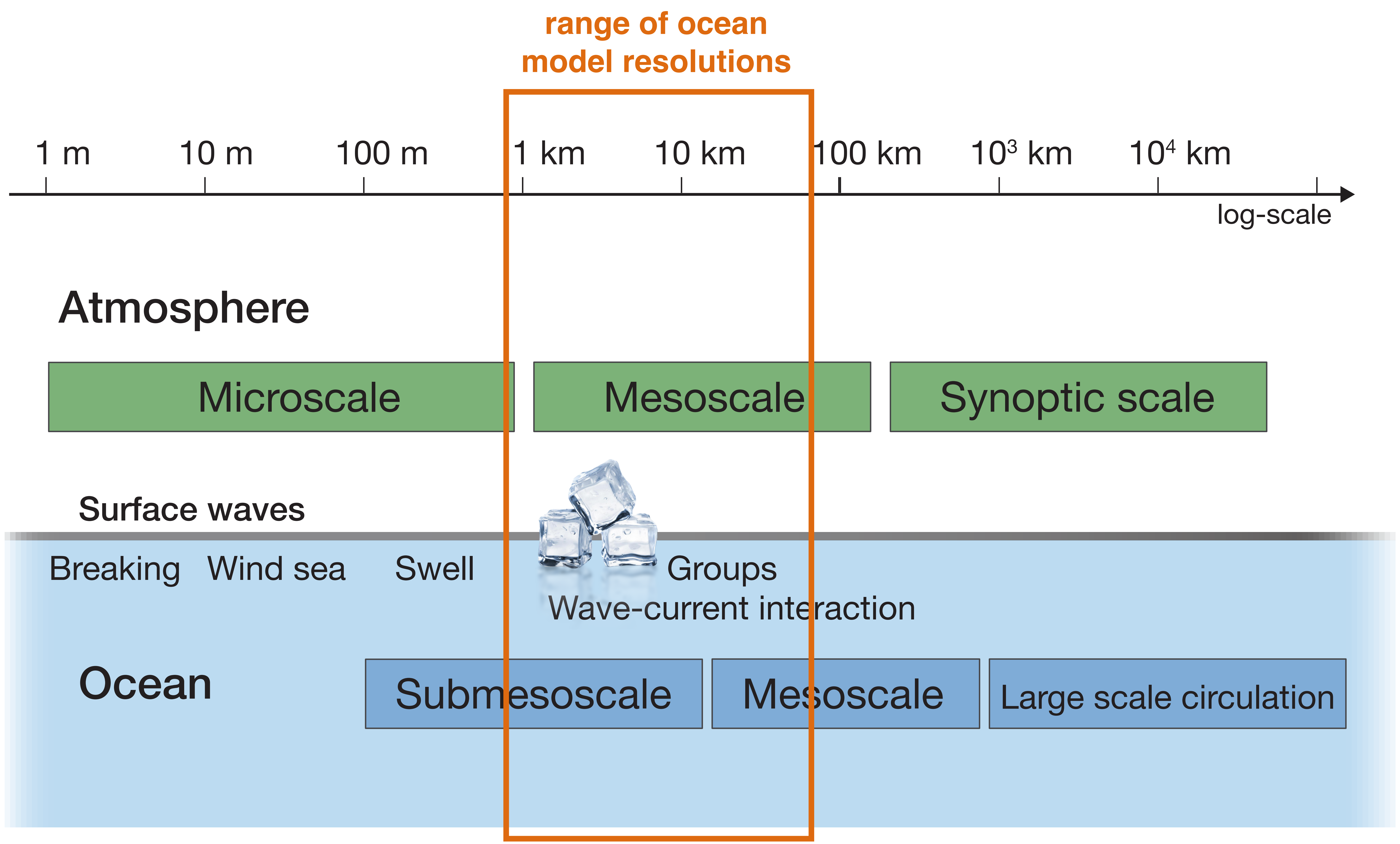
Adding Sea Ice: Storms co-locate with the Sea Ice Edge

Sea Ice gets more seasonal, and is dominated by the Marginal Ice Zone



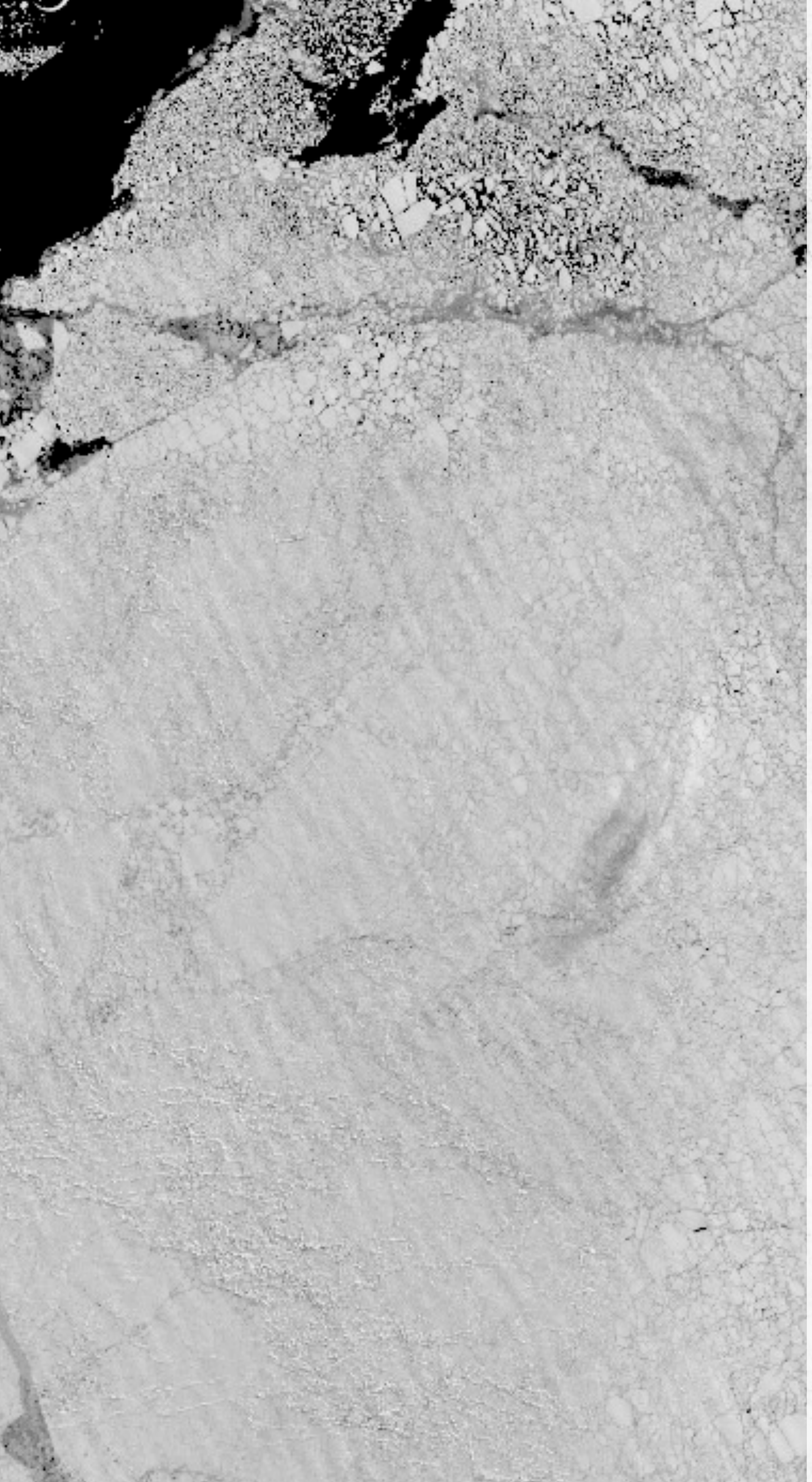
The **Marginal Ice Zone (MIZ)** is were ocean waves and sea ice coexist,
or, were sea ice is in proximity of to open water

Swell has a very non-local impact on the MIZ
We need to model swell



Models start to resolve scales at which ***complex dynamics*** can be important

- wave-current interaction
- wave-ice interaction
- wave groups
- wind waves in partially covered ice
- current-ice floe interaction in the MIZ
- forced ocean instabilities under leads
- forced atmospheric instabilities/clouds
- …



I. How to model surface waves in eddy-resolving ESMs
II. Particle-in-CelL for Efficient Swell - PiCELS
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How to model surface waves in eddy-resolving ESMs

3rd-generation spectral wave models

Wave action is solved in terms of space λ, ϕ, wave number *k* and direction θ

$$N(\lambda, \phi, k, \theta, t)$$

$$\frac{\partial N}{\partial t} + \nabla_x \cdot \dot{\mathbf{x}} N + \frac{\partial}{\partial k} \dot{k} N + \frac{\partial}{\partial \theta} \dot{\theta} N = \frac{S}{\sigma},$$

Conservation of wave action

$$\dot{\mathbf{x}} = \mathbf{c}_g + \mathbf{U},$$

Advection by the group velocity and currents

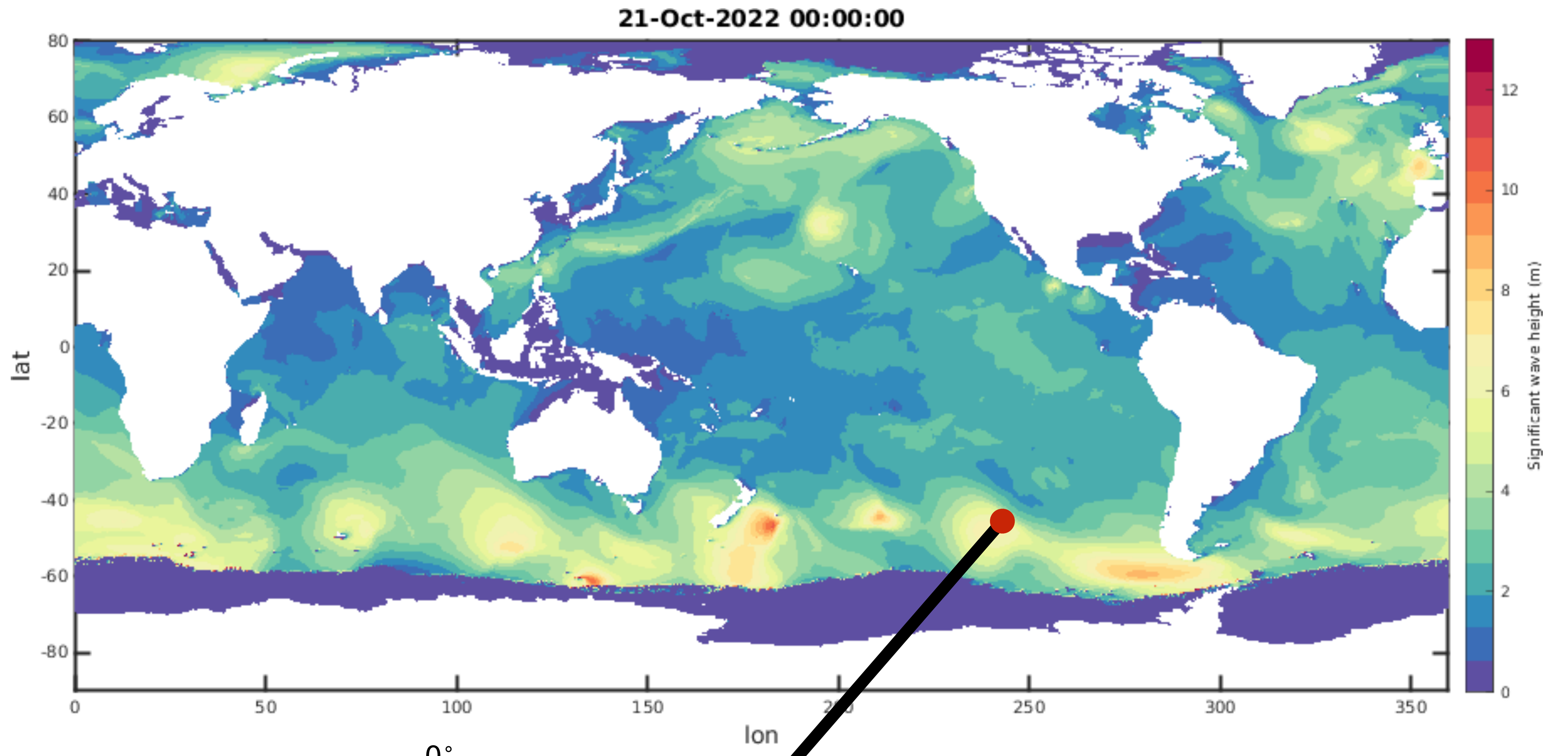
$$\dot{k} = -\frac{\partial \sigma}{\partial d} \frac{\partial d}{\partial s} - \mathbf{k} \cdot \frac{\partial \mathbf{U}}{\partial s},$$

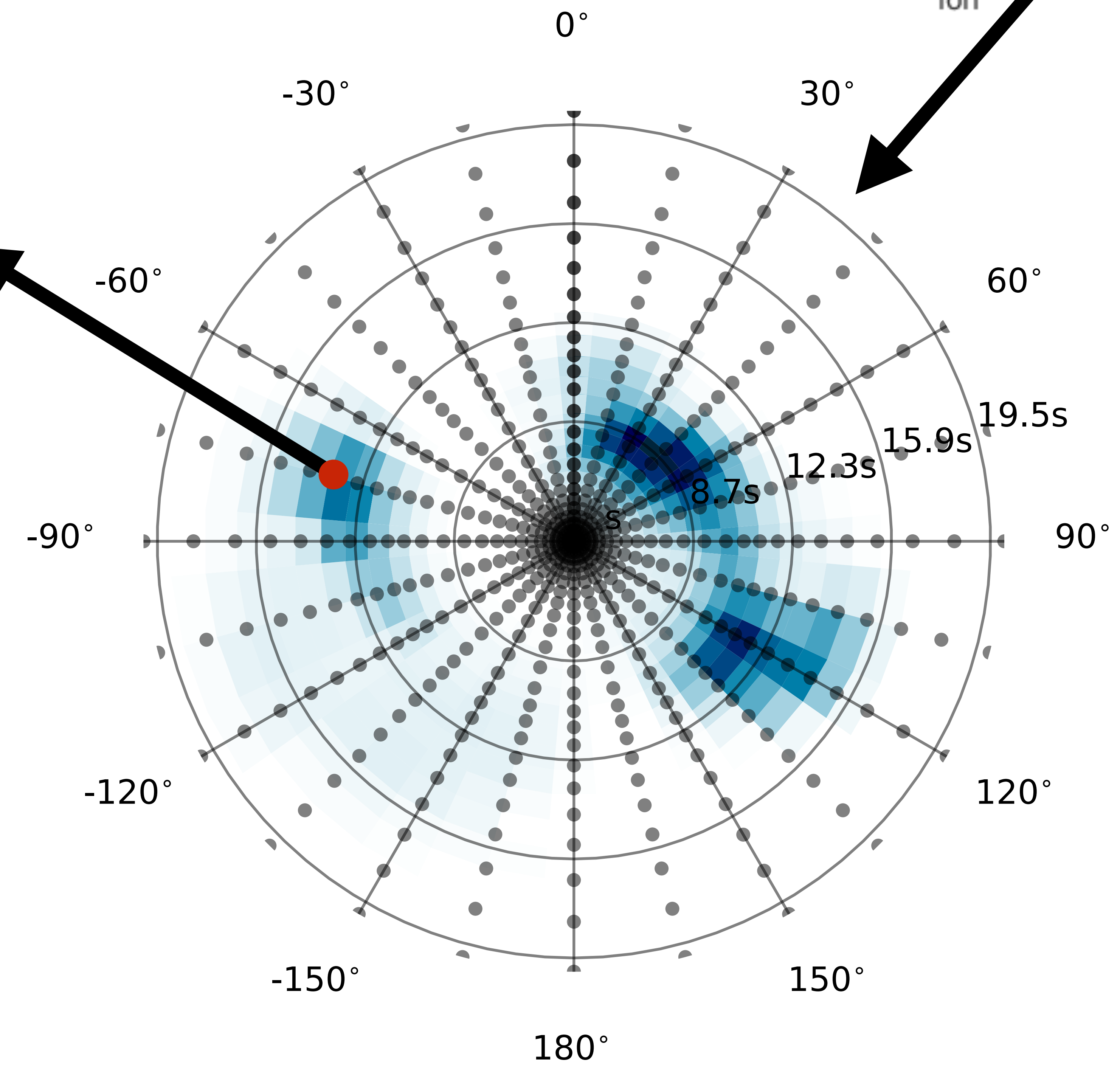
Change of wave number (s is in the direction of the angle)

$$\dot{\theta} = -\frac{1}{k} \left[\frac{\partial \sigma}{\partial d} \frac{\partial d}{\partial m} + \mathbf{k} \cdot \frac{\partial \mathbf{U}}{\partial m} \right]$$

Change of wave direction (m is perpendicular to s)

(WAM, 1984 - 1994, WAMDI Group, 1988, WaveWatch III, Tolman, 2006, ecWAM, ECMWF, 2024, SWAN)



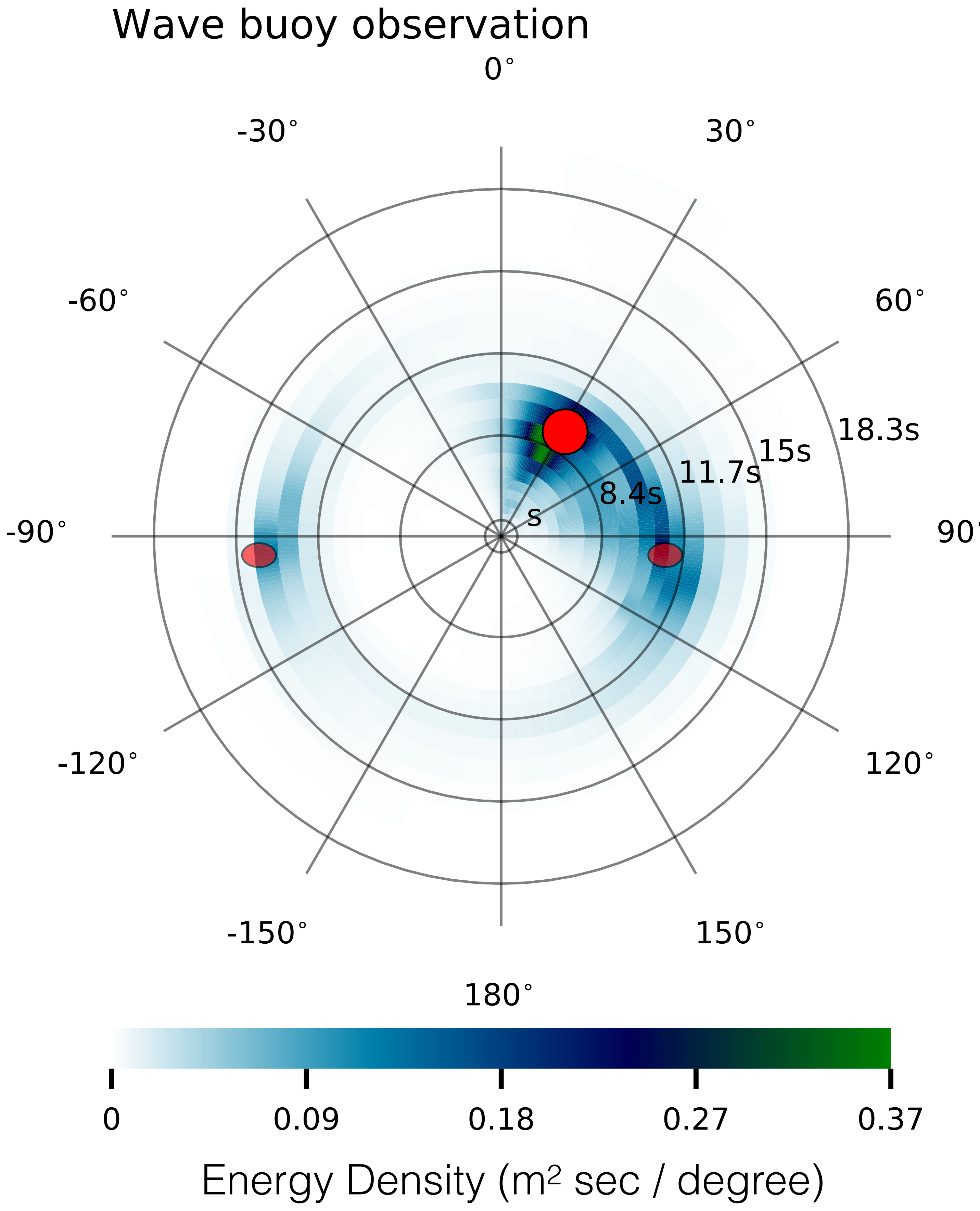


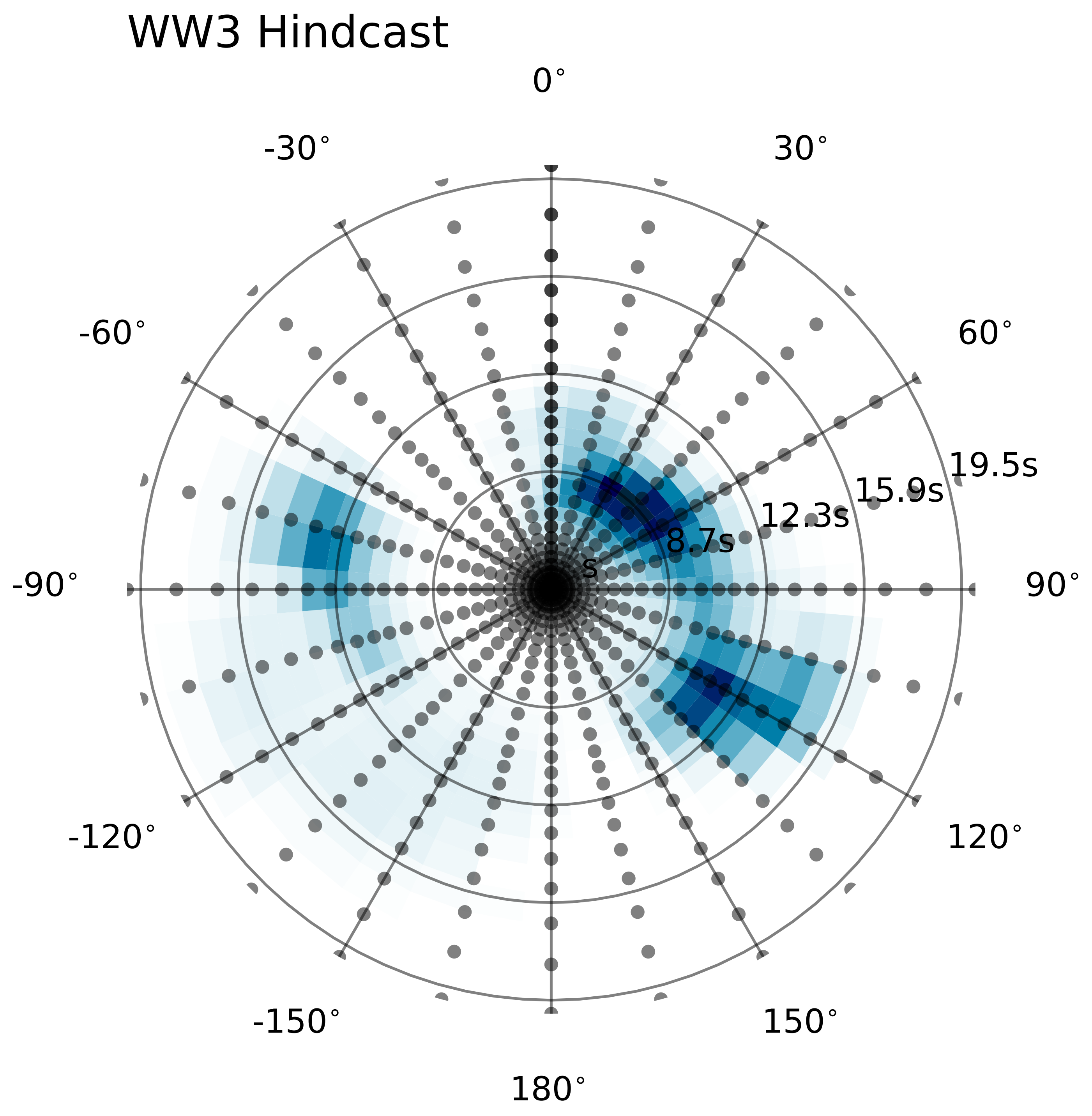
Spectral grid at each Spatial grid point

25 frequencies x 24 wavenumber

Why will we not use a spectral wave model in future Earth System models?

Directional wave spectra at Ocean Station Papa





- The information used for coupling is only **1-3% of the state vector**
- A **large state vector** and **interaction-terms** make spectral wave models **accurate tedetively slow**

Typical wave observations

approx. 6-12 variables

Spectral wave model discretize the wave action in frequency and direction:

about 600 variables

Why will we not use a spectral wave model in Earth System Models?

Spectral models are *too expensive* for global high-resolution integrations

Spectral Models in ESMs

- large state vector (~600)
- Spectral coupling may need larger overhead
- Accurate wave-wave interaction get even more expensive

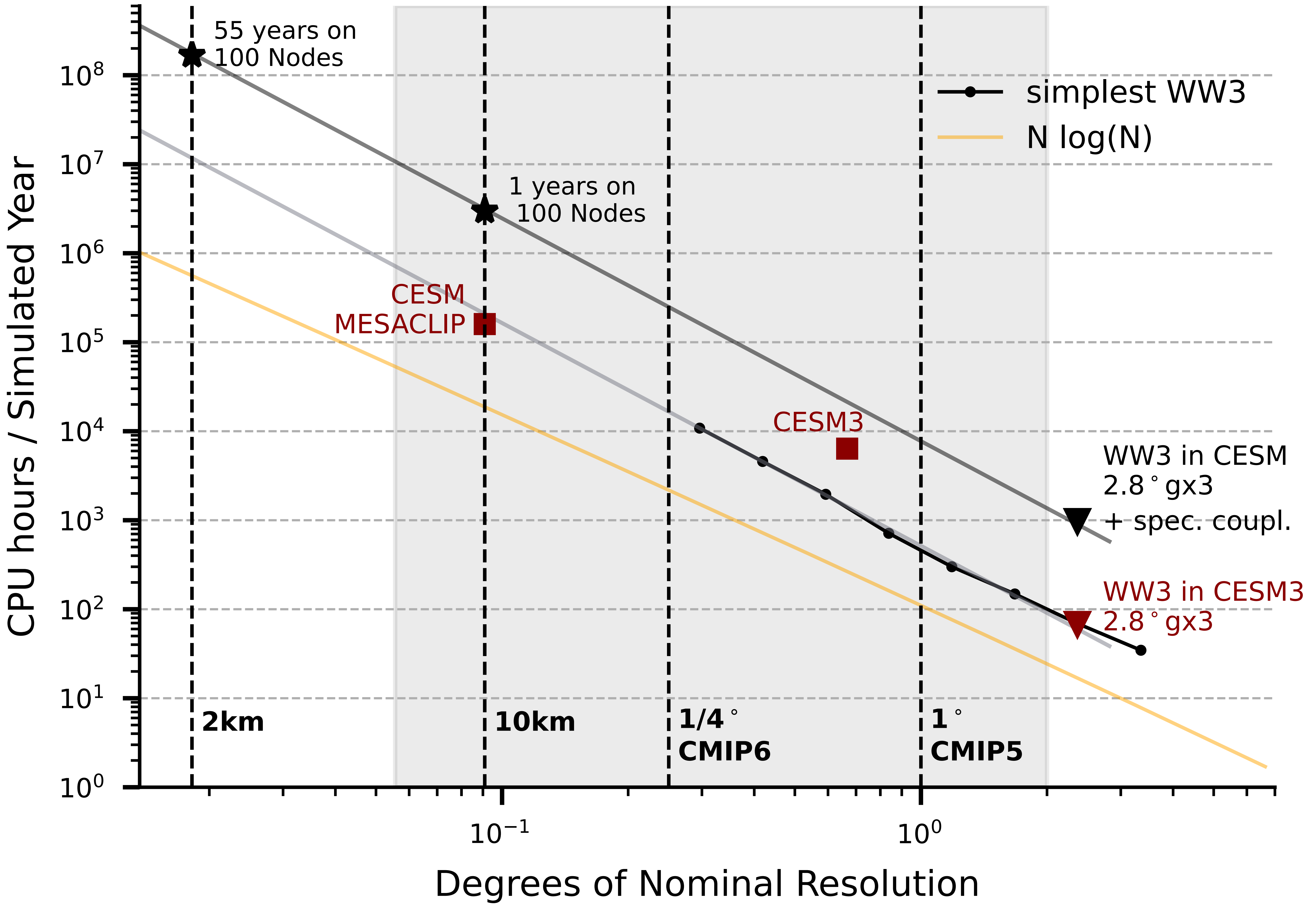
➡ WW3 on $2.8°$ runs at 1% of CESM3 total cost

➡ WW3 on $2/3°$ would cost 22% of CESM3

➡ WW3 on $1/10°$ would cost 130% of CESM MESACLIP

Is increasing complexity and cost justified for the gain in physical representation?

CPU hours per simulated year for a given ocean grid



Klaus Hasselmann’s vision

A wave model for climate models, not for wave modelers.

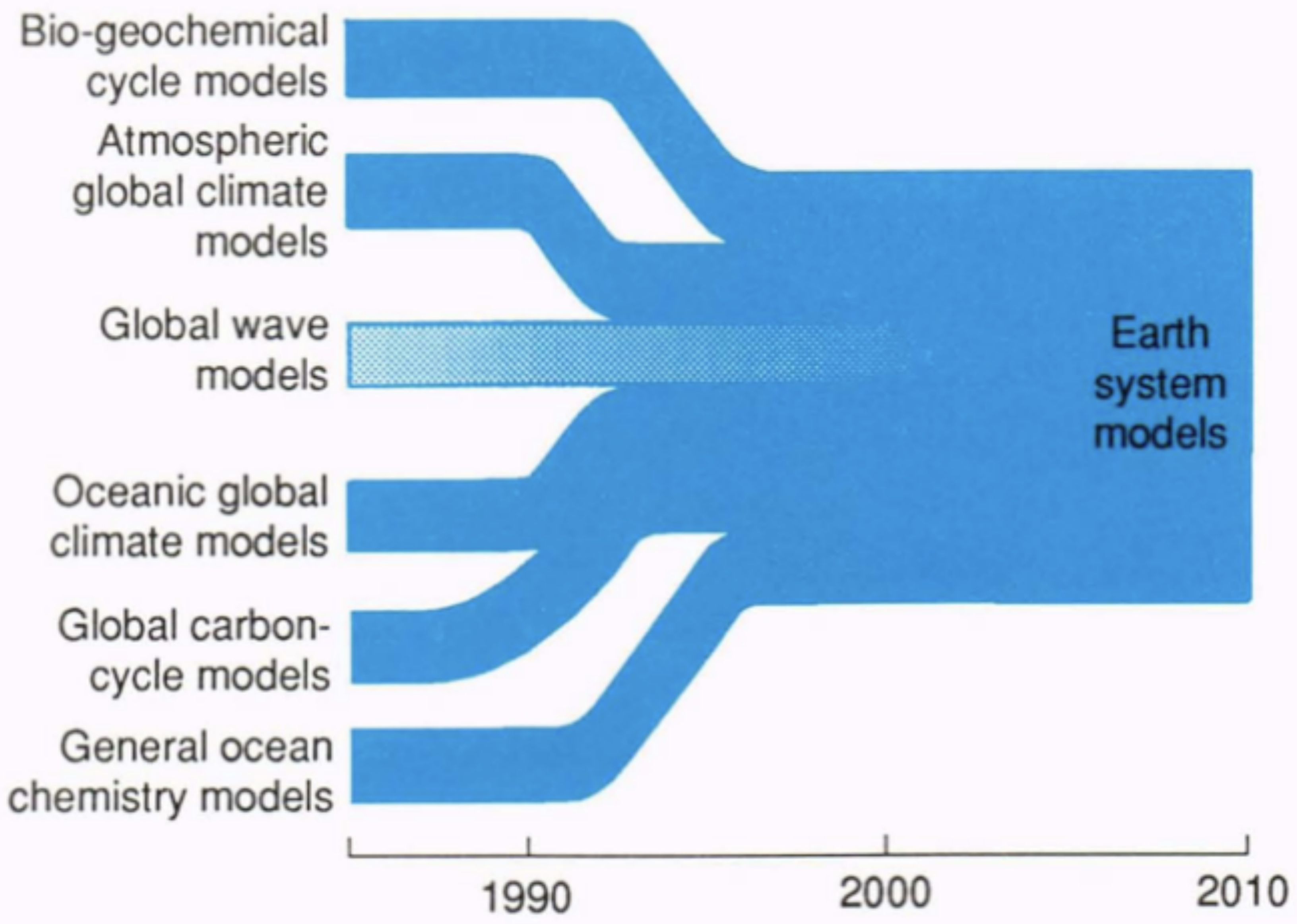


Figure 1. Future role of wave models as an essential coupling component for ocean–atmosphere–carbon-cycle models developed in the context of the World Climate and Global Change programs.

The future role of wave models as an essential coupling component for Earth system models in the context of global warming

“Waves, Dreams, and Visions" - (Hasselmann, 1990)

Constrains for *future* waves models in earth system models

1. **Moment-based metrics** of disequilibrium wind-sea and swell to **sufficient accuracy to drive 3-way coupling** between Atmosphere, Ocean, and Sea Ice
2. Stay **computational feasible** on the ocean grid resolution (1-3% of the total cost is common CESM practice)
3. **Easily scaleable to kilometer’s resolution** even on unstructured grids.
4. **Learn from remote sensing data**

≠ high skill in wave prediction on the weather forecast scale

Particle-in-CelL for Efficient Swell *PiCLES*

Enabling wave-coupling with Earth System Models

.. under review in JAMES

Momme Hell, Baylor Fox-Kemper, and Bertrand Chapron

NSF | NCAR Operated by UCAR

BROWN LOPS

WOODS HOLE OCEANOGRAPHIC INSTITUTION

A Lagrangian wave model on an Eulerian grid

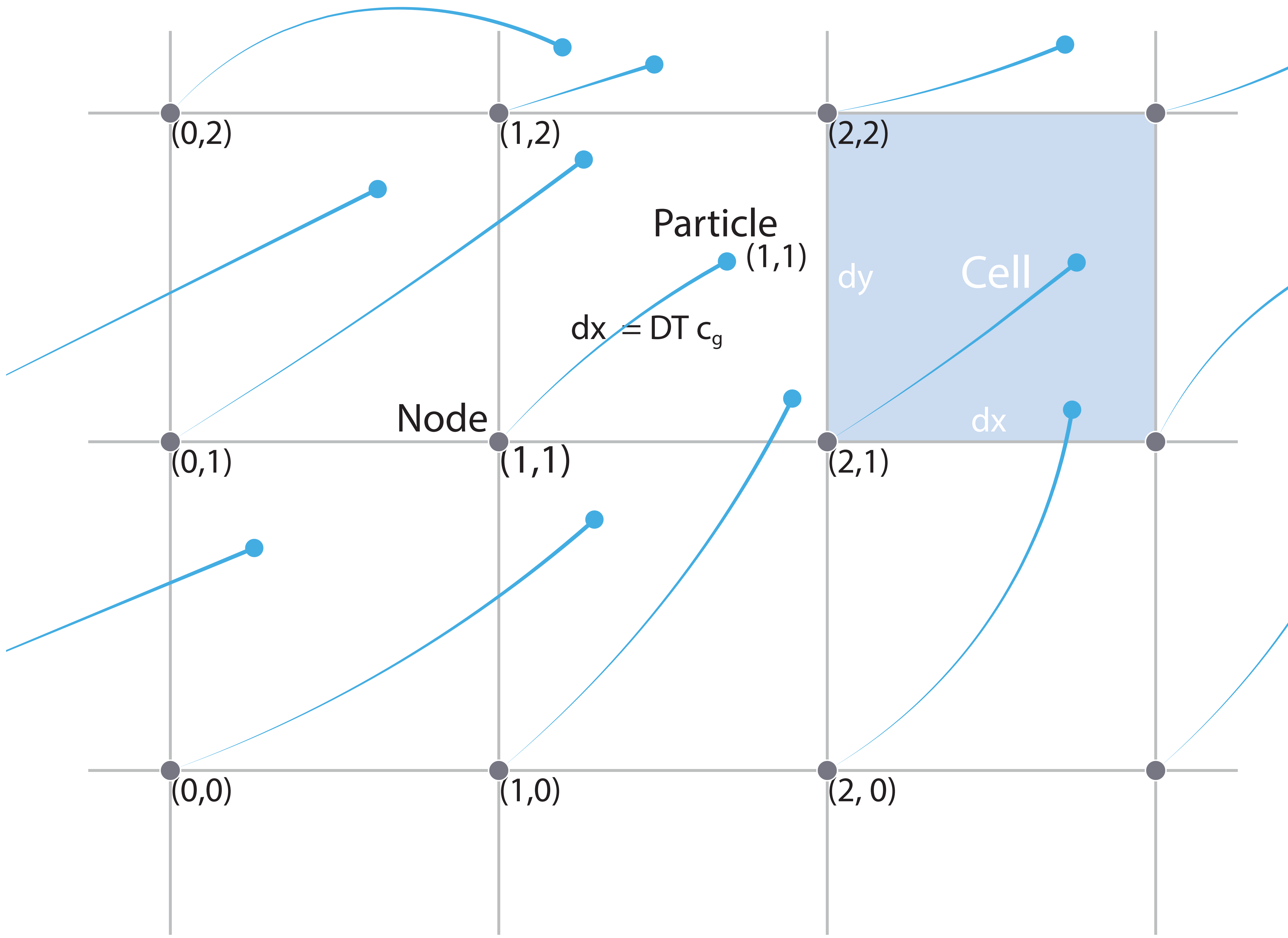
Particle-in-CelL for Efficient Swell *PiCLES*

- Solves the wave field along Lagrangian trajectories (particles) that are re-meshed periodically
- Each particle is a representative sample for energy & momentum of wave system
- Resolve the physics we know (propagation) and parametrize the rest

… designed for constrains of next-gen. ESMs

Trade accuracy for speed and convenience!

- Find alternative, low-dimensional model to **improve efficiency**
- Describe **sufficiently accurate** surface wave statistics for air-sea couplings in ESMs



Key Targets:

- Minimize particle interaction
- Written in julia
- Focus on open-ocean waves
- Good performance on GPUs

PiCLES numerics

Equations are solved along a particle trajectory

Conservation of wave action:

$$\frac{\partial}{\partial t}N + \frac{\partial}{\partial x_j}(\dot{x}_j\, N) + \frac{\partial}{\partial k_j}(\dot{k}_j\, N) = \frac{\mathcal{S}^E}{\sigma},$$

- neglecting currents
- integrating in (2D) wavenumber space
- forming equations for the total energy and momentum *(Kudryavtsev et al. 2021)*

Particle Equations

parameterized wave-wave interaction

Similar to WW3

$$\frac{d}{dt} ln\varepsilon = \sigma_p\, r_g\, \tilde{\mathcal{S}}^{cg} + \sigma_p(\tilde{I} - \tilde{D}),$$

$$\frac{d}{dt}\bar{c}^g_i = -\bar{c}^g_i\, \sigma_p\, r_g\, \tilde{\mathcal{S}}^{cg} + [\bar{c}^g_2, -\bar{c}^g_1]^T\, \sigma_p\, \tilde{\mathcal{S}}^{dir}$$

$$\frac{d}{dt}x_i = \bar{c}^g_i\,.$$

Parametrized change in direction

- Wave-wave interaction along the trajectory is parametrized

Particle state vector

$$\mathbf{p} = [\ \ln(\varepsilon),\ \bar{c}^g_1,\ \bar{c}^g_2,\ x,\ y\ ]^T$$

PiCLES numerics:

Lagrangian Step & Particle-in-Cell re-meshing

At each node (i,j):

(a) initialize(), if there is wind

t + Δt

(b) advance!()

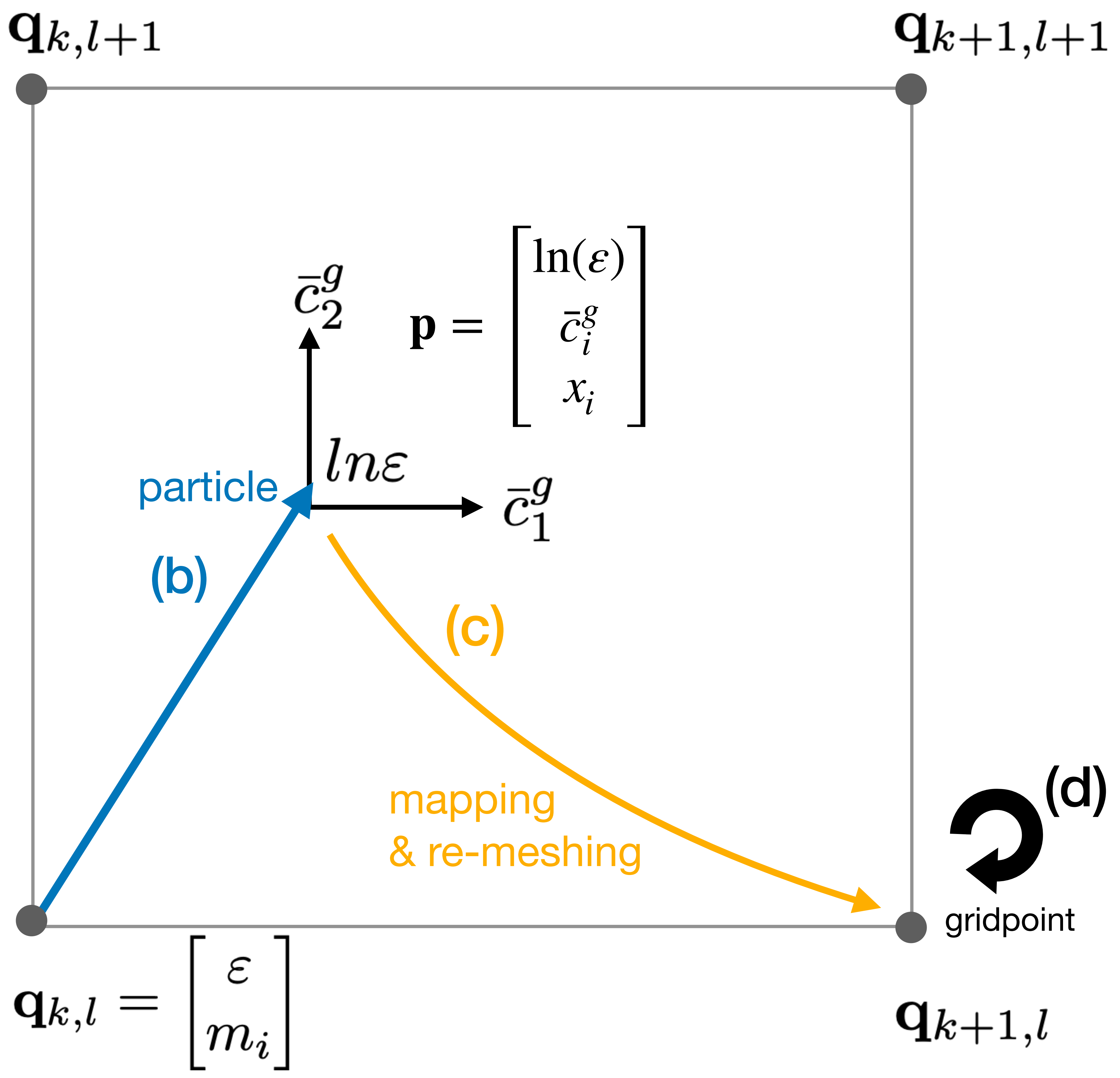
- if there is a particle, nothing otherwise

(c) remesh!()

- map **p** —> **q**
- State **S** += **q**

(d) reset!()

- map **q** —> **p**
- Initialize if there is wind or wave energy
- Set State **S** = 0



Particle state vector

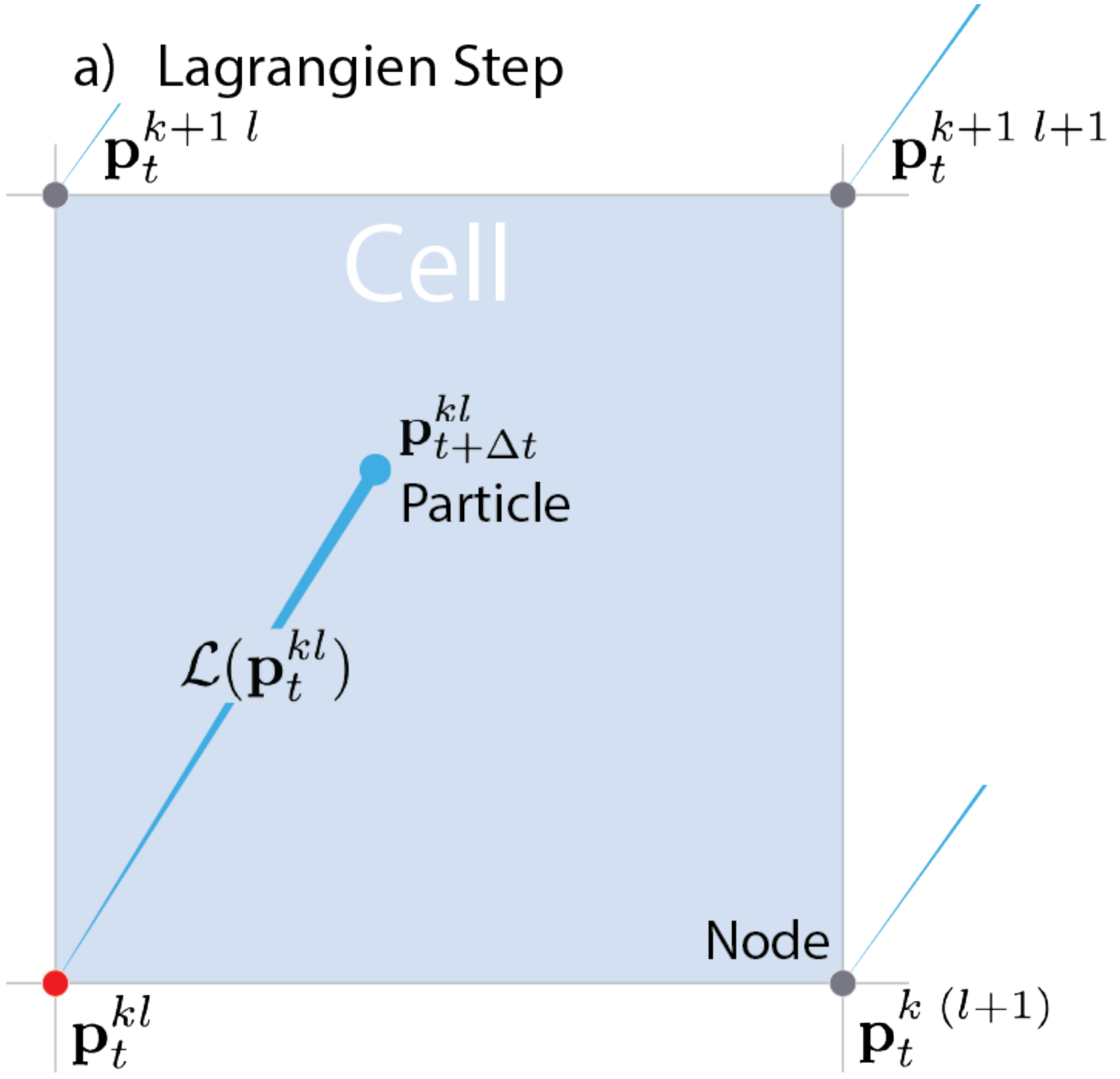
$$\mathbf{p} = \begin{bmatrix} \ln(\varepsilon) \\ \bar{c}_1^g \\ \bar{c}_2^g \\ x_1 \\ y_2 \end{bmatrix}$$

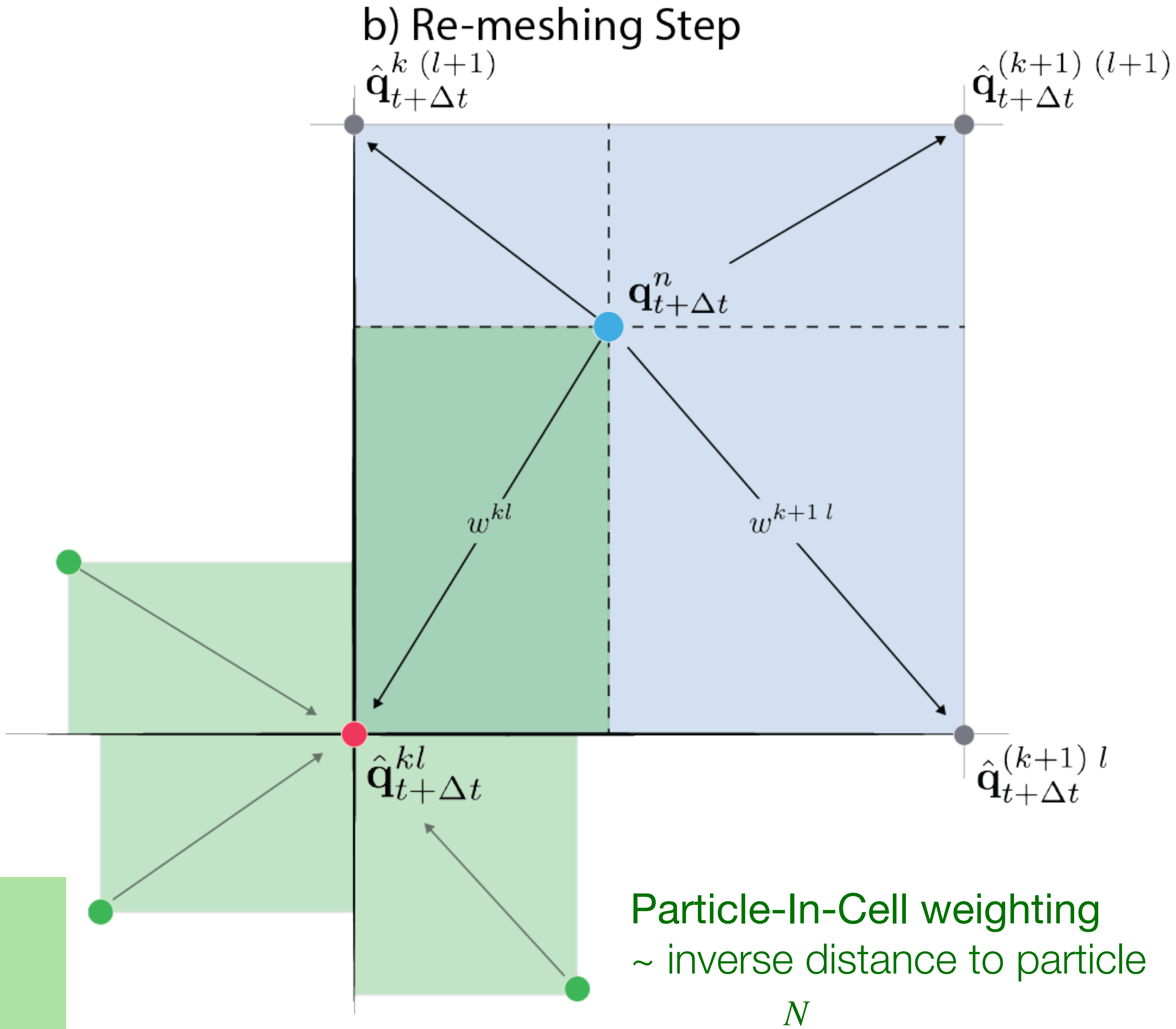
Grid state vector

$$\mathbf{q} = \begin{bmatrix} \varepsilon \\ m_1 \\ m_2 \end{bmatrix}$$

➡ You can **choose to represent** physics in **Lagrangian or Eulerian** space

Lagrangian Step & Particle-in-Cell re-meshing





➡ Mapping between **p** and **q** is the main trick to conserve energy and momentum

$$G(\mathbf{p}) \rightarrow \mathbf{q} \qquad \mathbf{p} = [\ \ln(\varepsilon),\ \bar{c}_1^g,\ \bar{c}_1^g,\ x_i,\ y_i\ ]^T$$

$$\mathbf{p} \leftarrow G^{-1}(\hat{\mathbf{q}}) \qquad \mathbf{q} = [\varepsilon,\ m_1,\ m_2\ ]^T$$

conserves energy and momentum

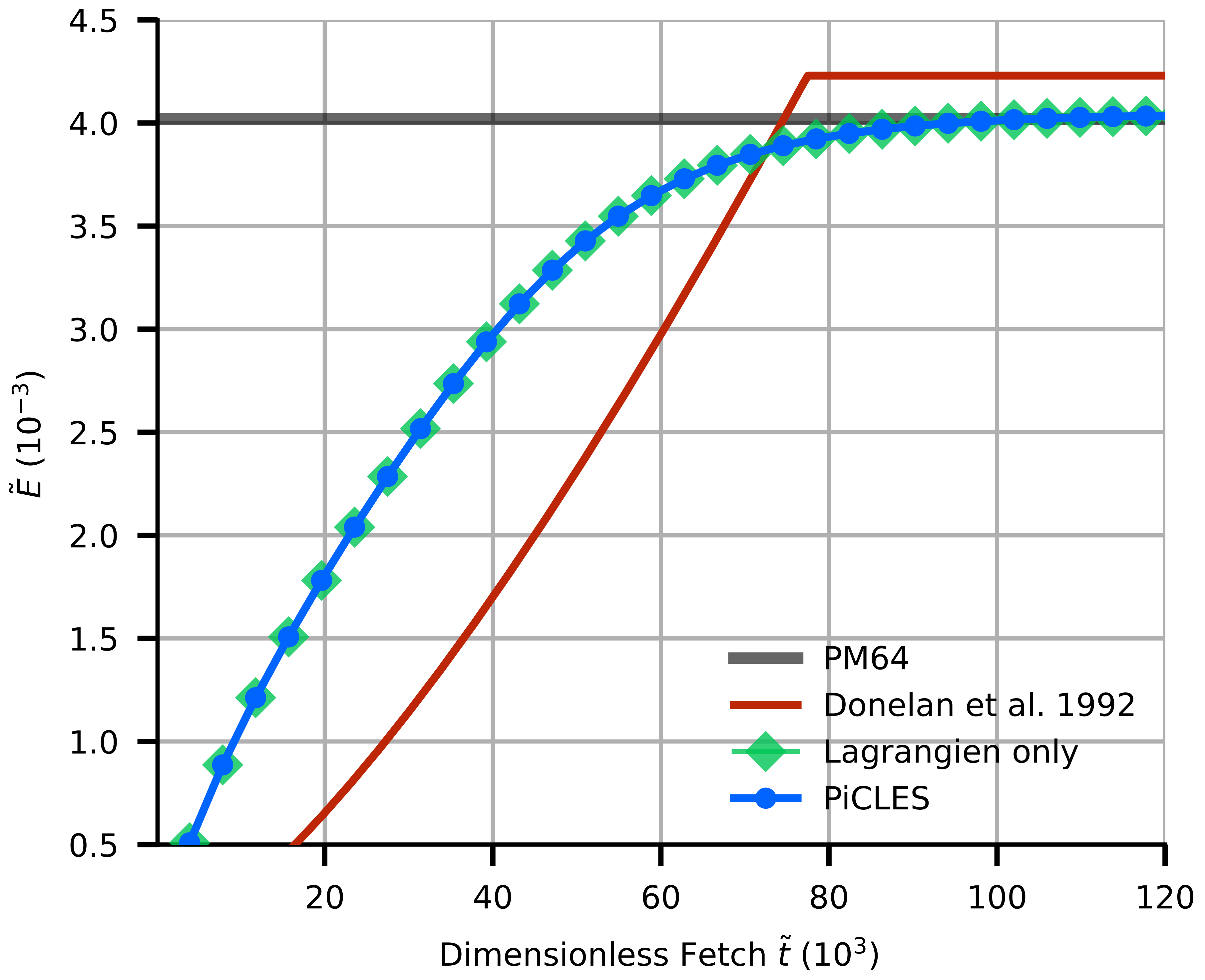
Particle-In-Cell weighting
~ inverse distance to particle

$$\hat{\mathbf{q}}_{k,l} = \sum_n^N w_n\ \mathbf{q}_n$$

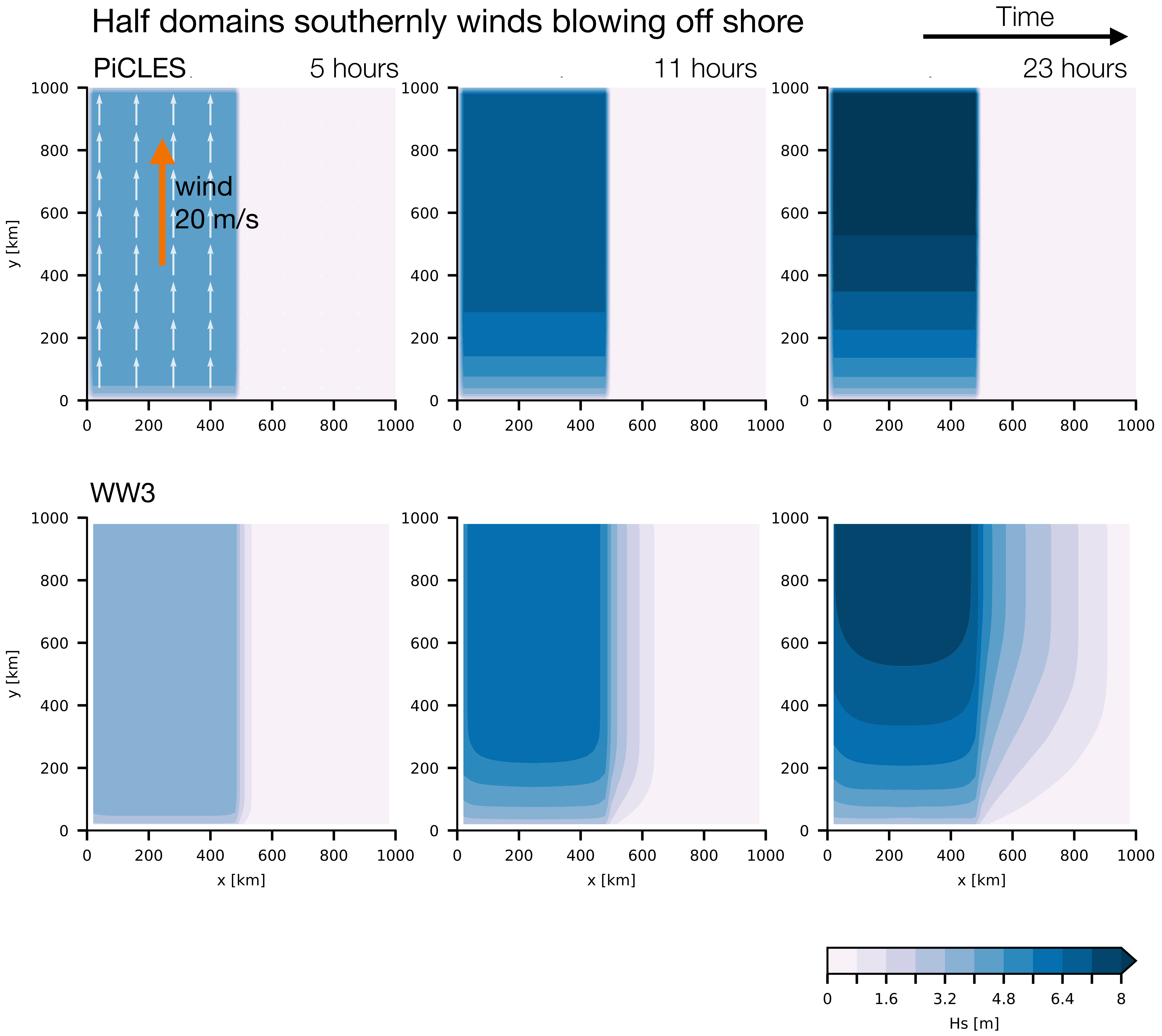
Accuracy | Static Fetches

- Lagrangian equations and PiCLES **reproduce wave-growth rates well** (to be optimized later)
- Regrinding scheme is **conservative and non-dispersive**

Dimensionless Energy $\tilde{E}$



Half domains southernly winds blowing off shore

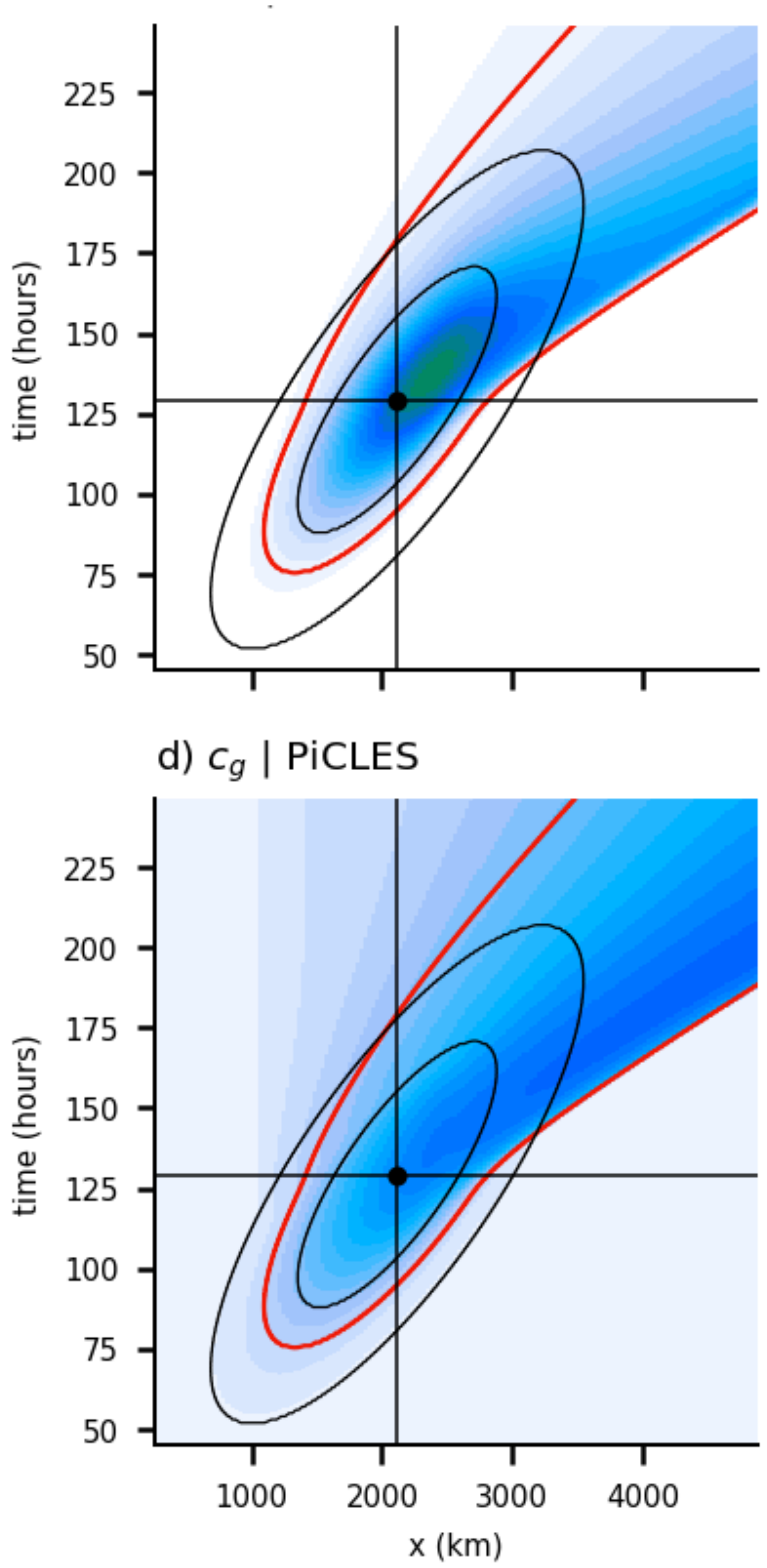


Accuracy | Idealized Moving Fetch Experiment

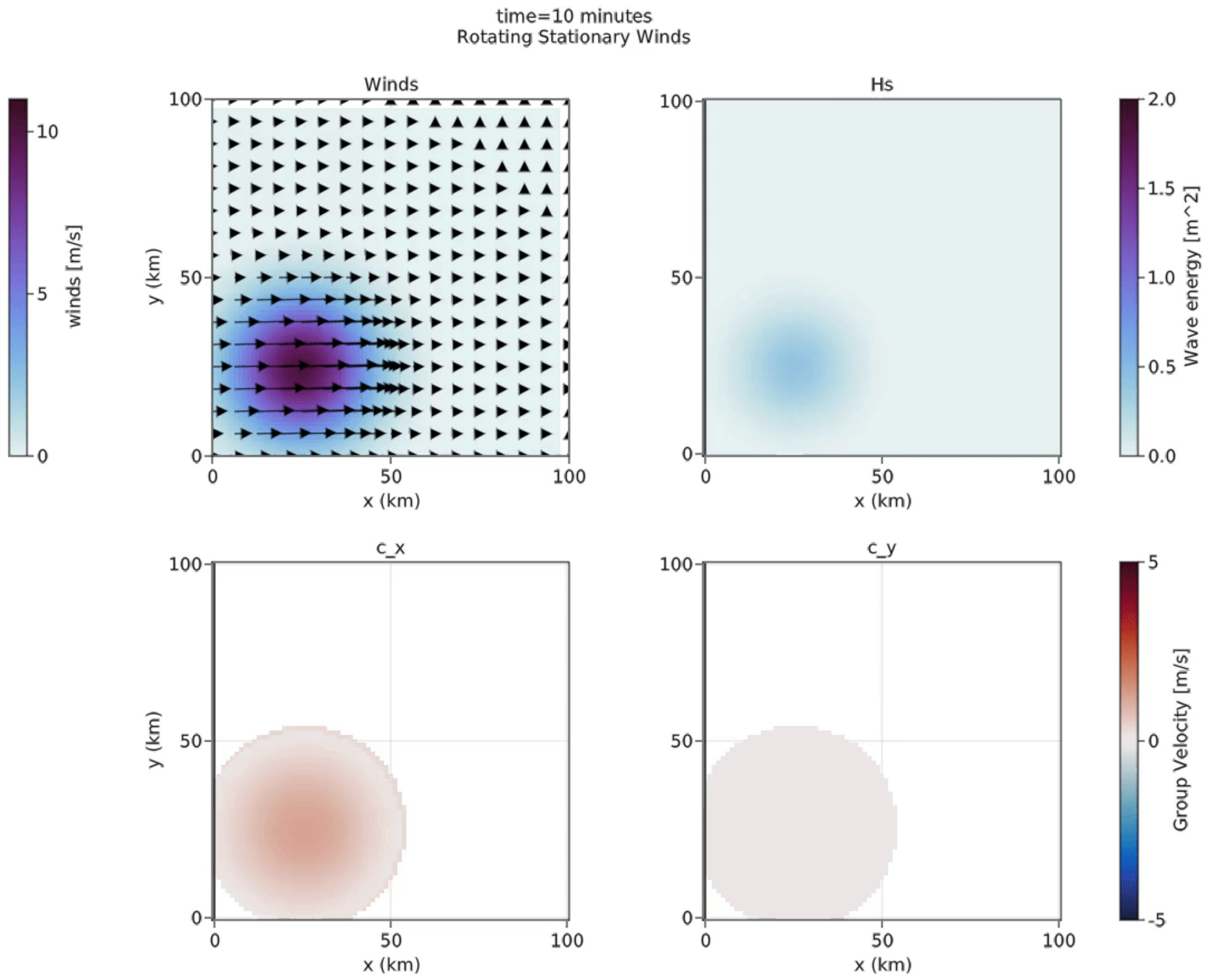
Skill in moment based metrics

Same idea as before:
Gaussian moving winds make waves

PiCLES **WW3 ST4 NL1** **WW3 ST4 NL4**



How to deal with these particle with dynamic winds?



Main Caveats:

Discretization in wave partition, rather then frequency and direction

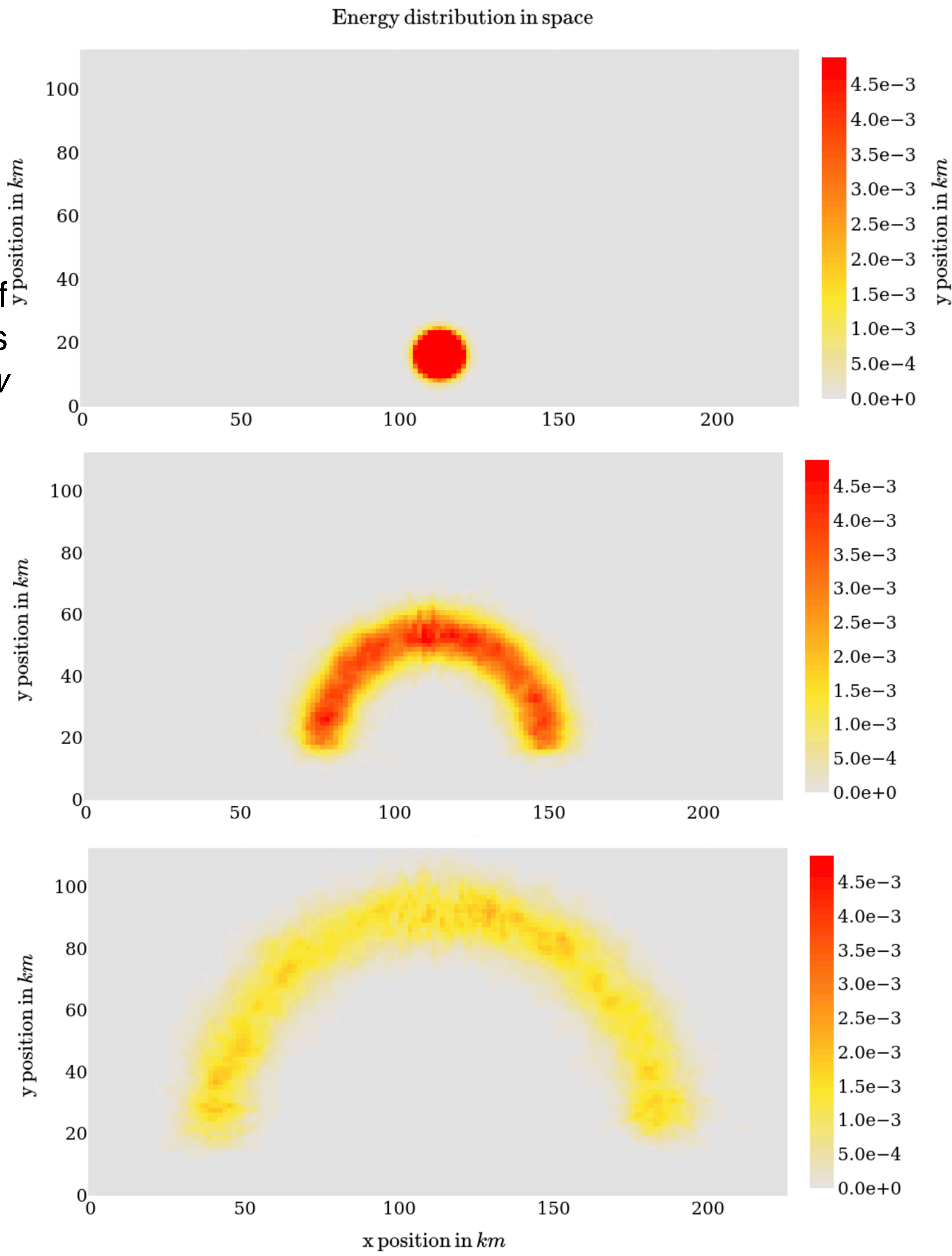
-> require to **invent a new set of algorithms for particle-particle interaction** (partition-partition interaction:

- How to decide between wind-sea and swell?
- How to superimpose wave partitions?
- How to describe their interactions?

Next steps: Propagating swell by superposition of wave partitions

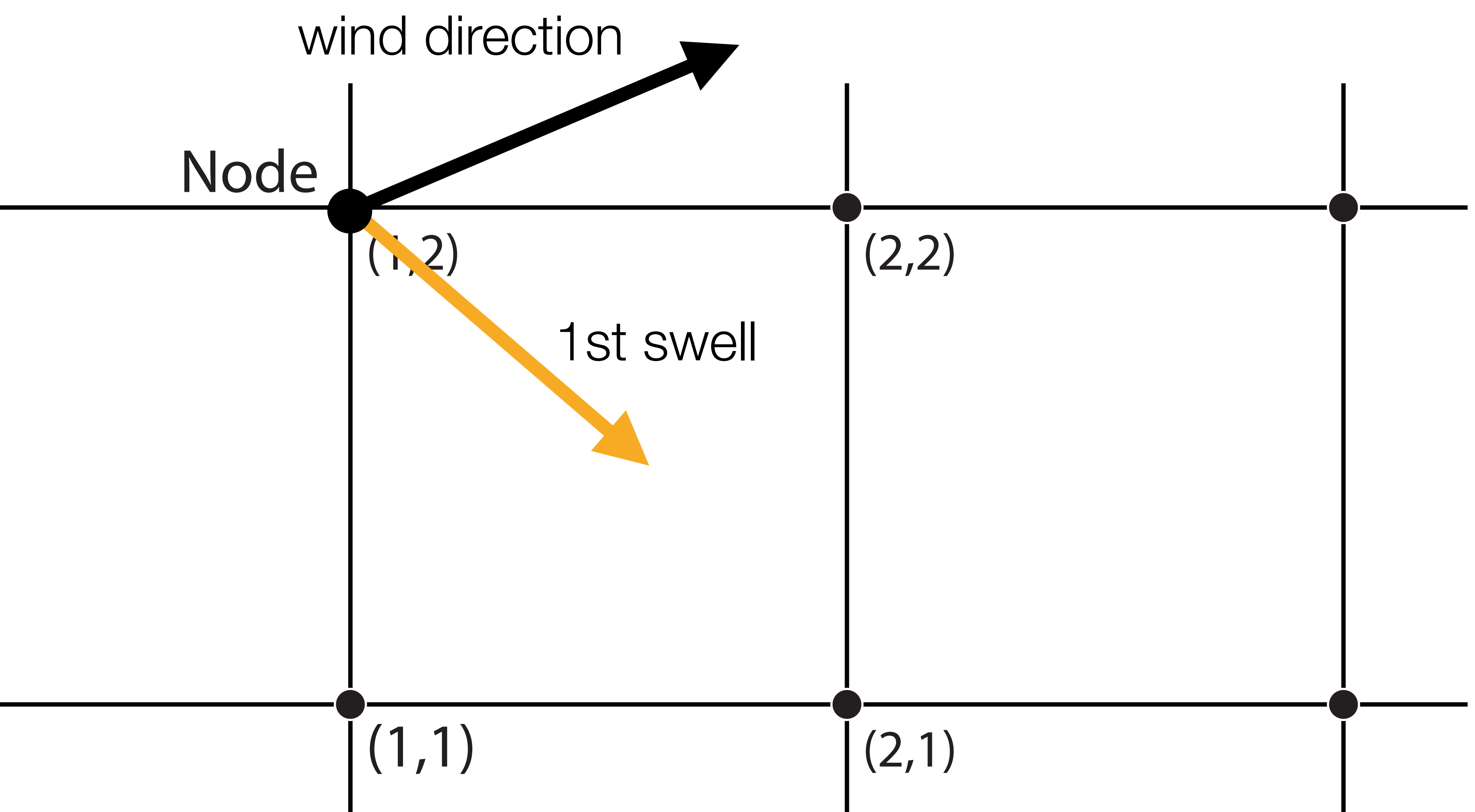
Geometrical optics behavior of resampled swell particles

Sequential importance resampling of particle-in-cell for swell dynamics
Protin et al 2025, under review



Each node has multiple particles

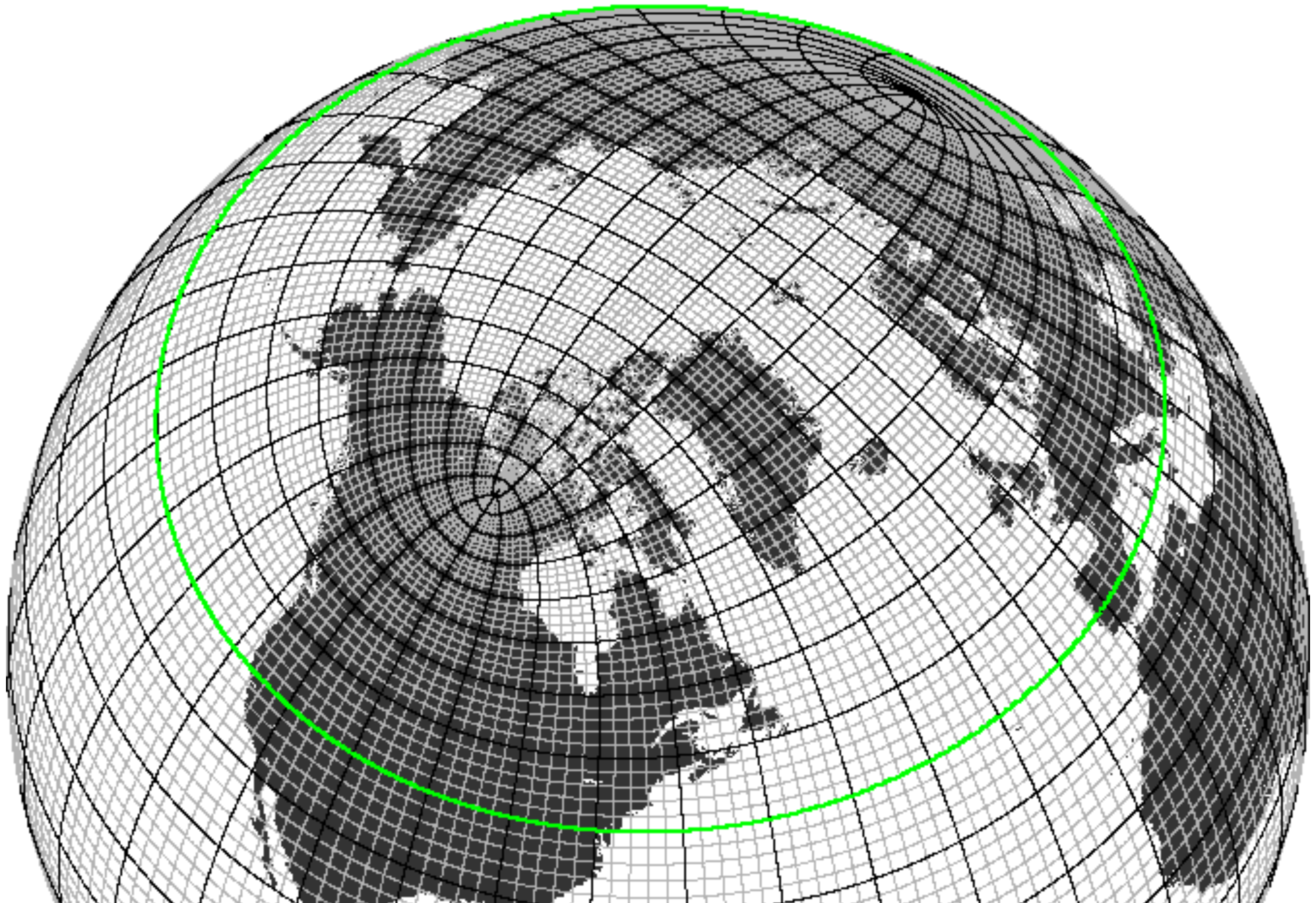
Wind sea:	1 x 5	energy, cg_x, cg_y, x, y
Swell I:	1 x 5	energy, cg_x, cg_y, x, y, + travel time
Swell II:	1 x 5	energy, cg_x, cg_y, x, y, + travel time
Swell III:	1 x 5	energy, cg_x, cg_y, x, y, + travel time

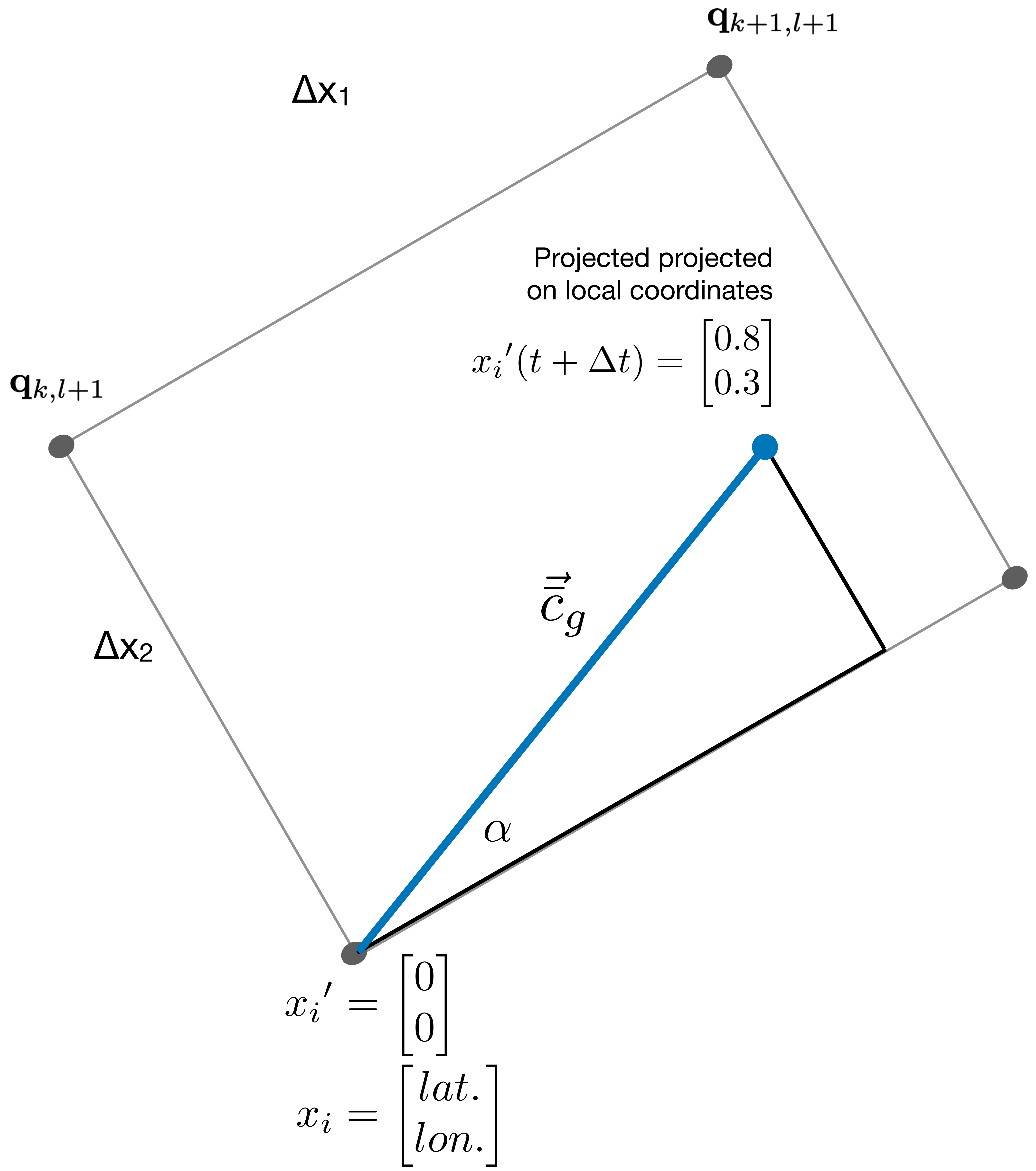


Next steps: Moving to other grids

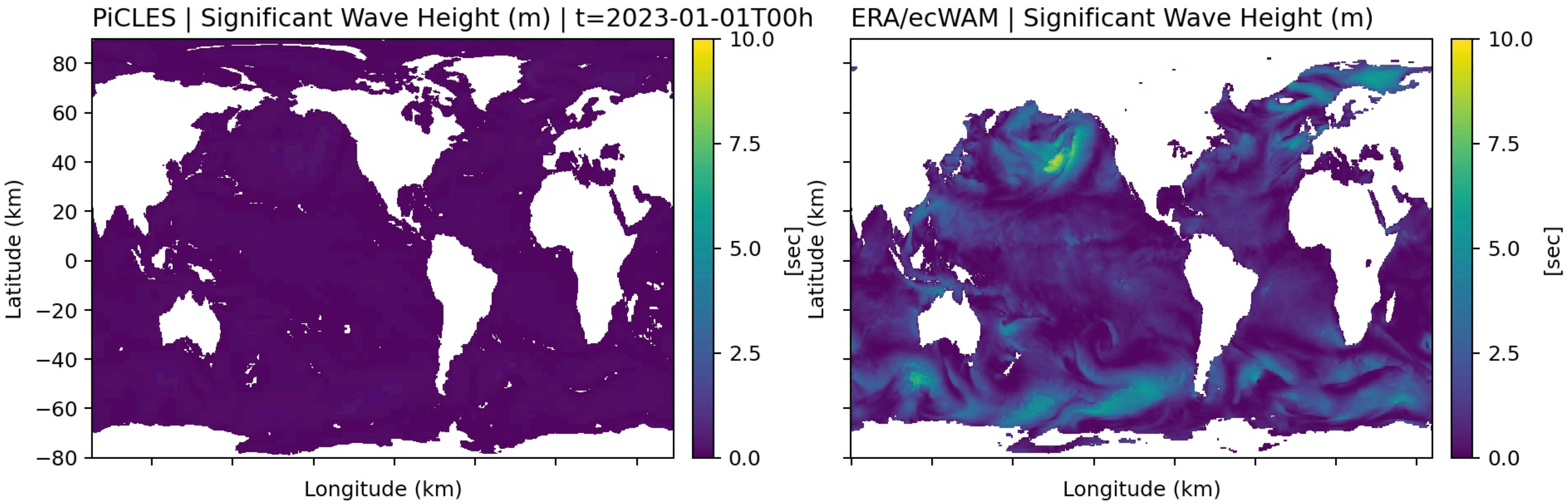
Re-meshing in non-cartesian coordinates

- Velocity tendency terms are calculated in SI units (m/s) but propagation is projected on local (•)' coordinates
- In rectangular grid, the position is the weight!
- Other geometries may just have more complex weight functions
- There is (a to be quantified) error for varying grid sizes.





First test runs on global tri-polar (MOM6) grid



Weak Scaling Tests I Out-running WW3

PiCELS will enable routine use of waves for air-sea coupling in high-resolution Earth System Models

Thanks to D. Bailey and G. Marques

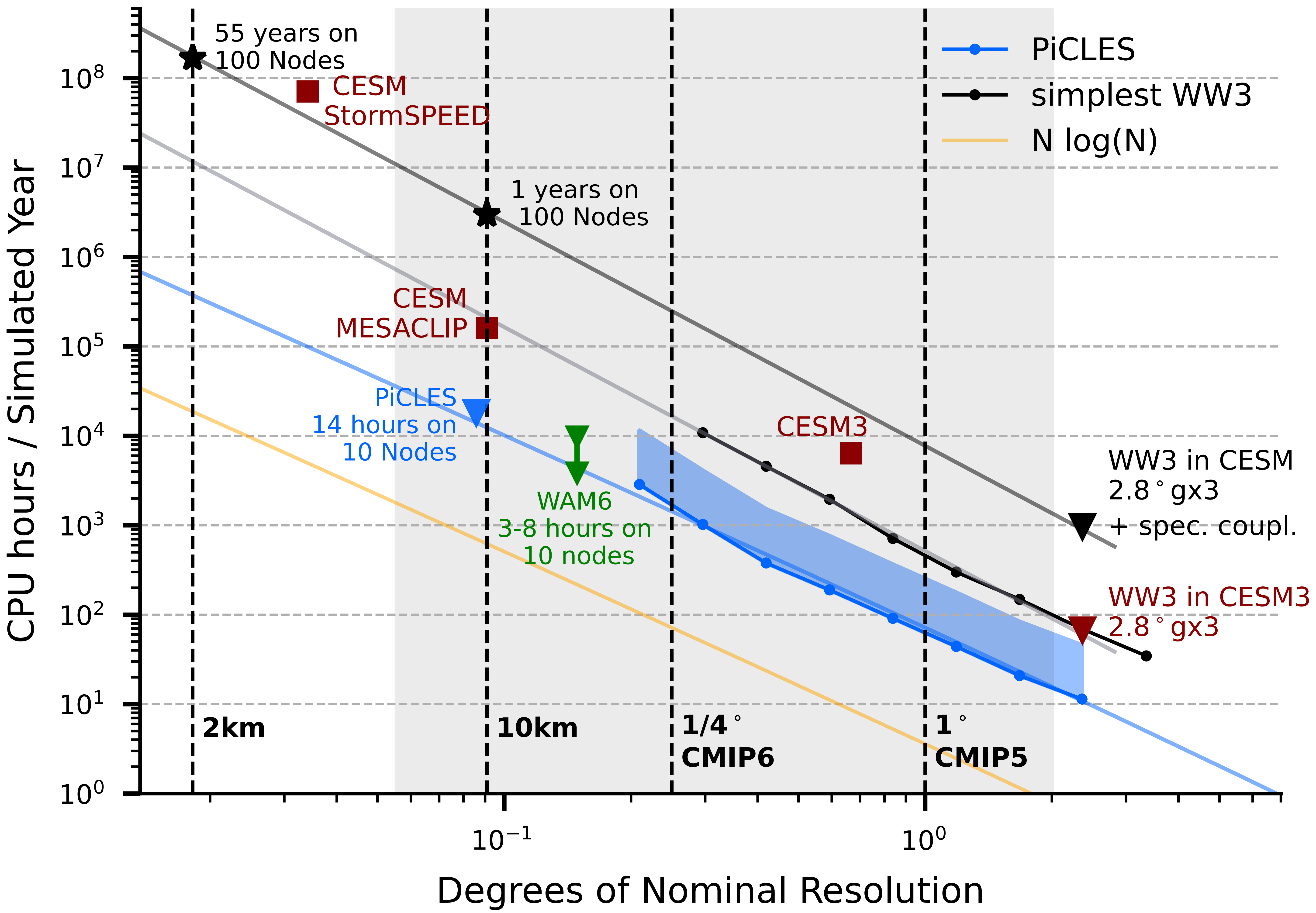
Spectral Models in ESMs

- Large state vector (~600)
- S_{nl} can be expensive
- WaveWatch III resolution in CESM is currently reduced to 2.8°

PiCLES:

- small state vector (about 5 - 20)
- runs on MOM6 ocean grid and time step
- can be well optimized for GPUs

CPU hours per simulated year for a given ocean grid



Performance

- *current* PiCLES is $\mathcal{O}(10)$ faster then **WW3** ***without overhead***
- PiCLES is about $\mathcal{O}(100)$ faster then **WW3** ***with spectral coupling***
- PiCLES would cost ~11% of CESM MESACLIP

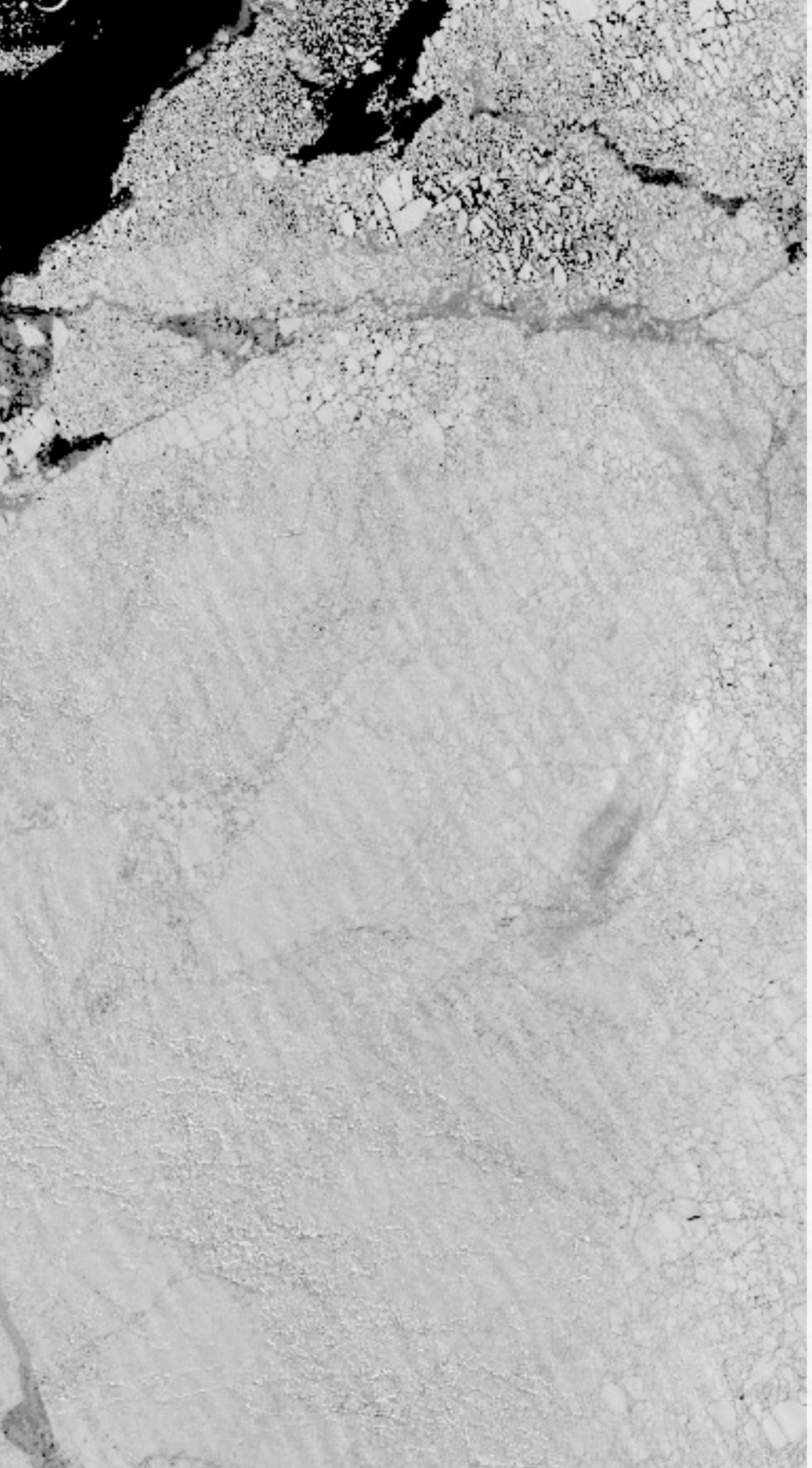
The future is PiCLES!

Steps towards a stand-alone wave model

1) Dispersion, Diffusion, and Refraction
2) Multi-layer & Merging rules
3) Optimize allocations
4) Determine time stepping limits

Toward an ML-driven model for air-sea exchange

- cheap and adjustable wave-information for ML-driven parameterizations in an ML-native language
- An improved representation of the interface



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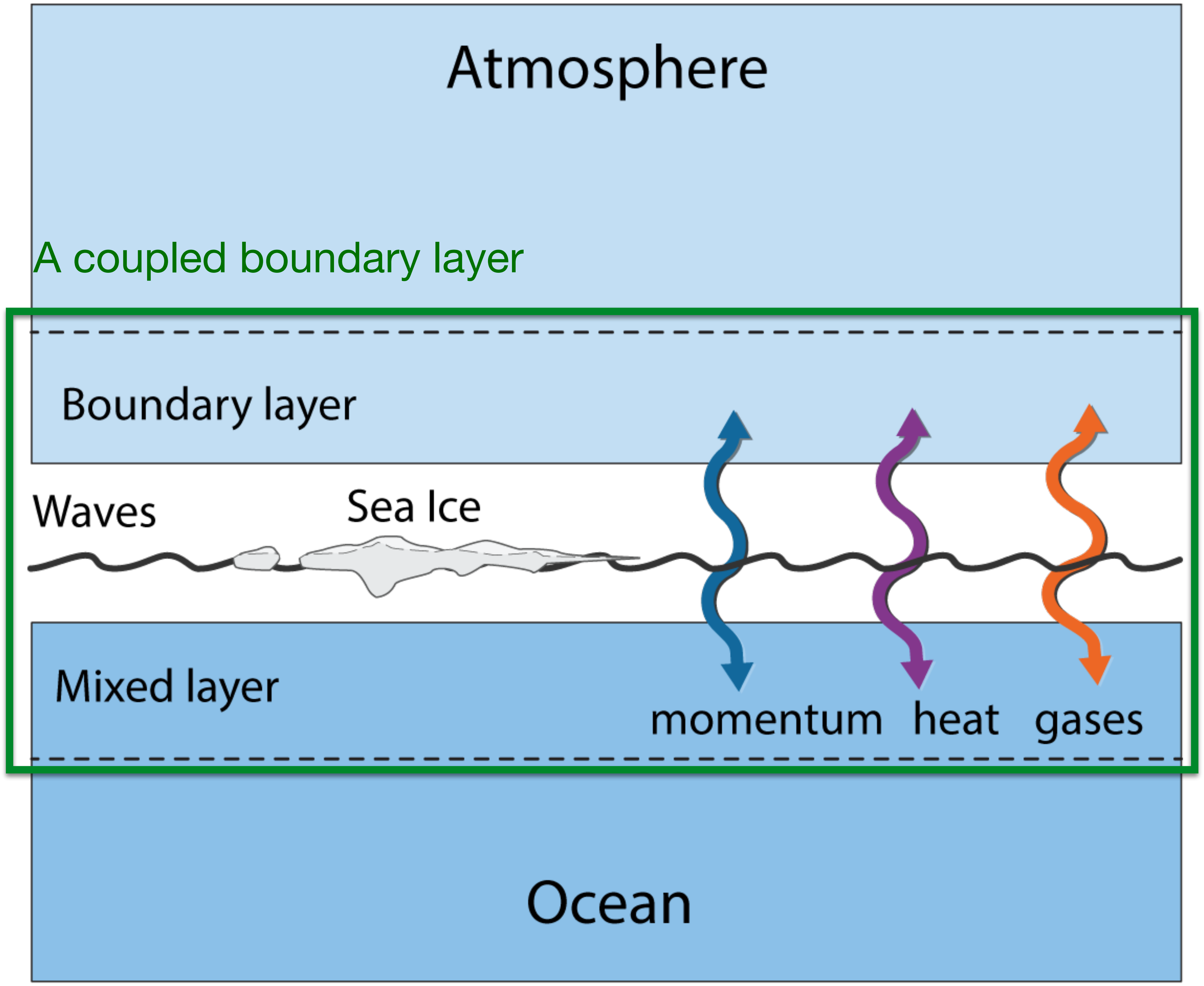
Grid box of an earth system model



Air-Sea Fluxes should generally depend on the wave spectrum, but

When do we need ***wave-based*** parameterizations?

When are ***wind-based*** parameterizations sufficient?

$$\tau = \rho_a c_d \left|\bar{\mathbf{u}}_a - \bar{\mathbf{u}}_o\right|(\bar{\mathbf{u}}_a - \bar{\mathbf{u}}_o)$$

$$C_D(S(\theta, f, t), u_{10}, L_M)$$

2D wave spectrum

We need a modeling infrastructure where we can test and quantify those impact

Current practice for sea state-dependent parameterizations

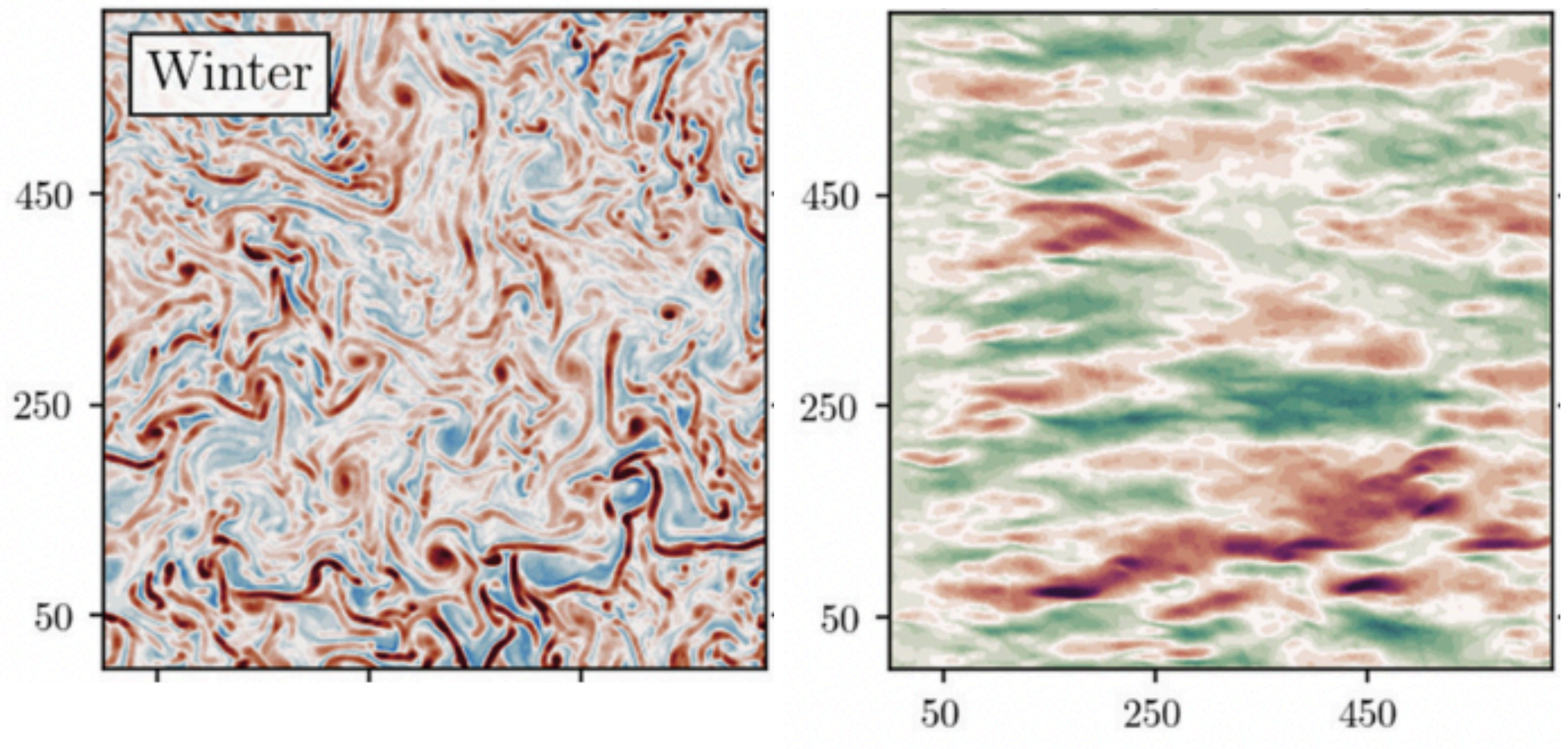
Process	Reference (and there in)	required wave variable
Atmosphere		
Gas transfer	Reichl & Deike 2020, Brumer et al. 2017, e.g.	H_s, f_p
Wave breaking	Romero 2019, Sutherland and Melville 2013, e.g.	c_p, saturation spectrum m_4, wave groups (spectral width)
Sea spray through wave breaking	Monahan et al. 1986, Fairall et al. 2009, Mueller and Veron 2009, Barr et al 2023 e.g.	H_s, c_p, mean squared slope m_2
Surface Drag	Sauvage et al. 2023, Patton et al. (2019), Porchetta et al. (2019),	wave age vector $(\mathbf{c}_p, \mathbf{u}_{10})$, steepness= $H s f_p$
Ocean		
Stokes Drift	Webb & FK 2011, Li et al 2016	$\mathbf{u}^s \approx F(m_3)$, sec. 1.4
Wave-current interaction	possibly Wang et al (under revision, U2H map)	2D wave spectrum, $S(f, \theta; f_p, \alpha_j, \bar{\theta})$, eq. 1.13
Marginal Ice Zone		
Sea ice breaking	Williams et al. (2013), Horvat (2022)	peak wave number, Hs and m_3
	Horvat & Tziperman 2015, 17, Roach, 2019, Cooper (2022)	1D Spectrum
	Ardhuin (2016)	Directional spectrum
Wave attenuation in Sea ICE	Liu et al. 2020 e.g.	$F(f, \theta)$

Simulated wave-current interaction on the submeso and mesoscale scale

(Boas et al. 2020)

sub-mesoscale currents

Significant wave height modulation



How much do **small scale gradients in Hs** effect Stokes Drift and other processes?

Remote Sensing shows many small-scale dynamics at play!

Current practice for sea state-dependent parameterizations

Atmosphere		
Process	Reference (and there in)	required wave variable
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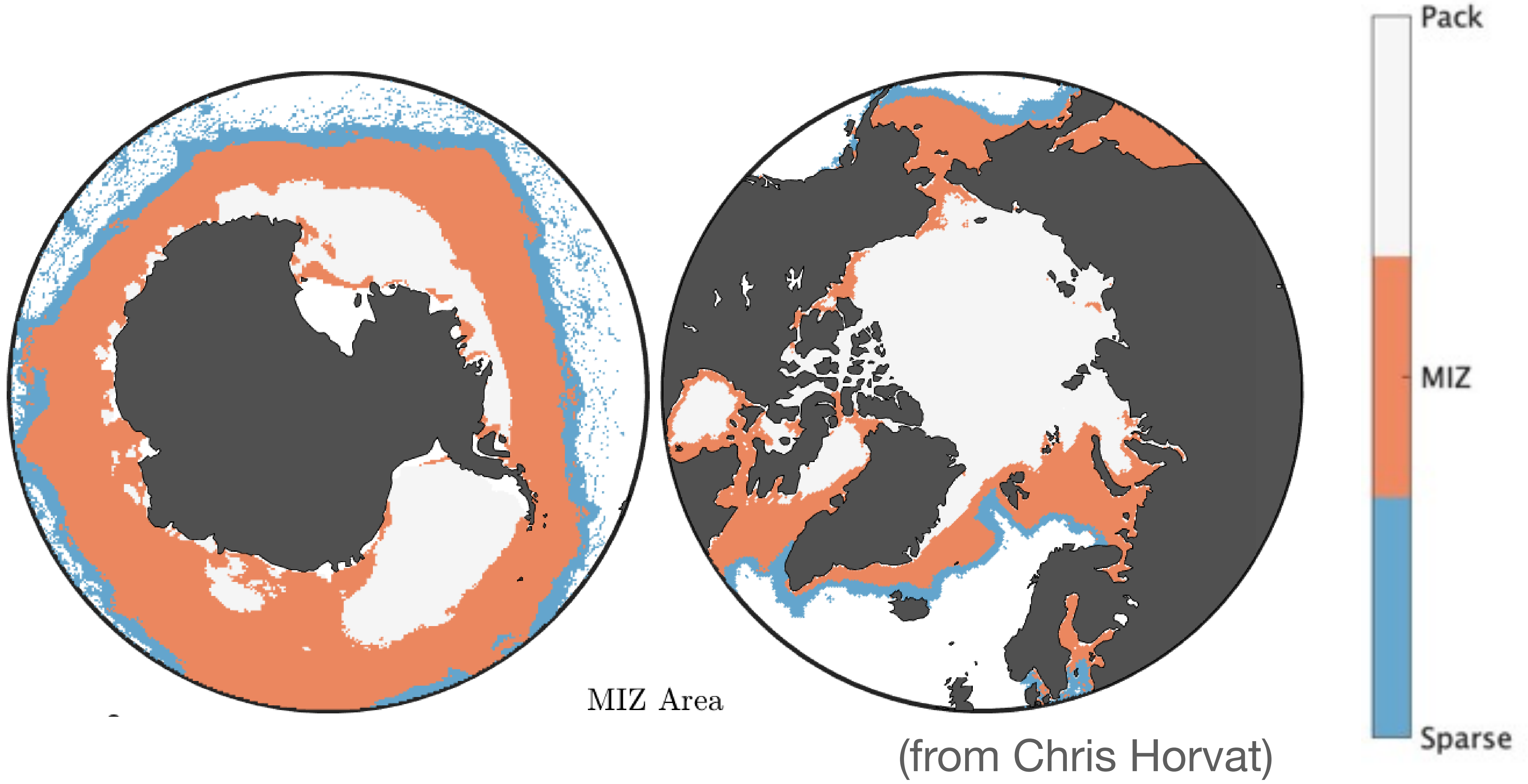
Wave-current interaction	possibly Wang et al (under revision, U2H map)	2D wave spectrum, $S(f, \theta; f_p, \alpha_j, \bar{\theta})$, eq. 1.13
Marginal Ice Zone		
Sea ice breaking	Williams et al. (2013), Horvat (2022)	peak wave number, Hs and m_3
	Horvat & Tziperman 2015, 17, Roach, 2019, Cooper (2022)	1D Spectrum
	Ardhuin (2016)	Directional spectrum
Wave attenuation in Sea ICE	Liu et al. 2020 e.g.	$F(f, \theta)$

Southern Ocean Marginal Ice Zone
20-60% of ice extent

Large discrepancy in the MIZ between CMIP6 models, likely due to wave forcing



(from Chris Horvat)

Swell has a very non-local impact on the MIZ
We need to model swell

Current practice for sea state-dependent parametrizations

mostly based on spectral moments

Atmosphere

Process	Reference (and there in)	required wave variable
Gas transfer	Reichl & Deike 2020, Brumer et al. 2017, e.g.	H_s, f_p
Wave breaking	Romero 2019, Sutherland and Melville 2013, e.g.	c_p, saturation spectrum m_4, wave groups (spectral width)
Sea spray through wave breaking	Monahan et al. 1986, Fairall et al. 2009, Mueller and Veron 2009, Barr et al 2023 e.g.	H_s, c_p, mean squared slope m_2
Surface Drag	Sauvage et al. 2023, Patton et al. (2019), Porchetta et al. (2019),	wave age vector $(\mathbf{c}_p, \mathbf{u}_{10})$, steepness= $H s f_p$
Ocean		
Stokes Drift	Webb & FK 2011, Li et al 2016	$\mathbf{u}^s \approx F(m_3)$, sec. 1.4
Wave-current interaction	possibly Wang et al (under revision, U2H map)	2D wave spectrum, $S(f, \theta; f_p, \alpha_j, \bar{\theta})$, eq. 1.13
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Moment based Parameterizations

assume deviations from standard spectral shapes have no leading-order effect *(Webb & Fox-Kemper 2011, 2015)*

$$m_n = F_n(H_s, f_p)$$

H_s and f_p are essentially fetch parameters

Spectral moments:

$$m_n = \int_0^\infty \int_0^{2\pi} f^n \, S(\theta, f) \, df \, d\theta$$

$S(\theta, f)$ 2-dimensional Spectrum

either from parametric functions, or modeled by full spectral models

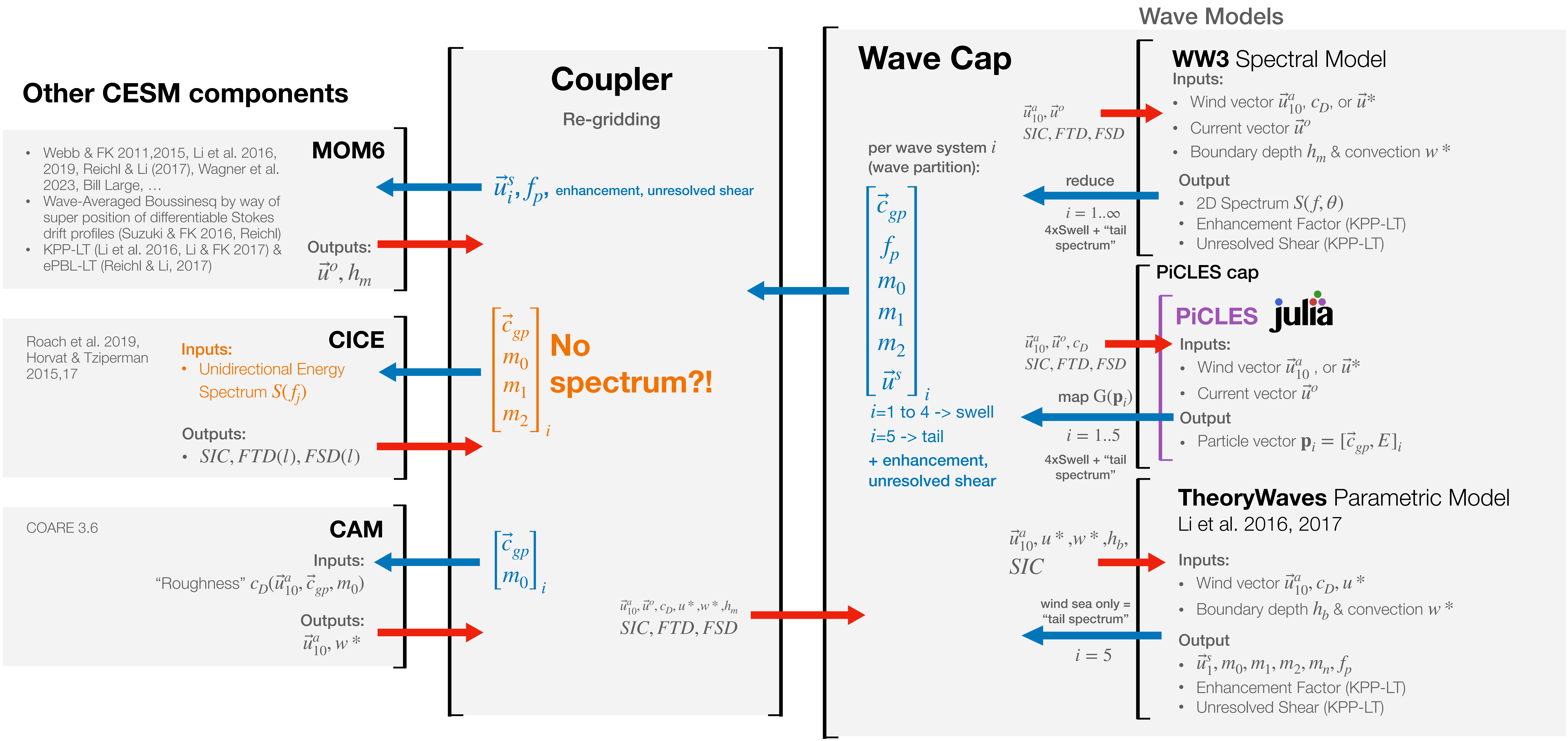
I assume coupling effects can <u>always</u> be simplified based on moments in eddy resolving models.

Full-spectrum based parameterizations

assume details in the spectrum matter to leading order and spectra can be modeled to that detail

Towards a standard, unified wave-coupling in CESM

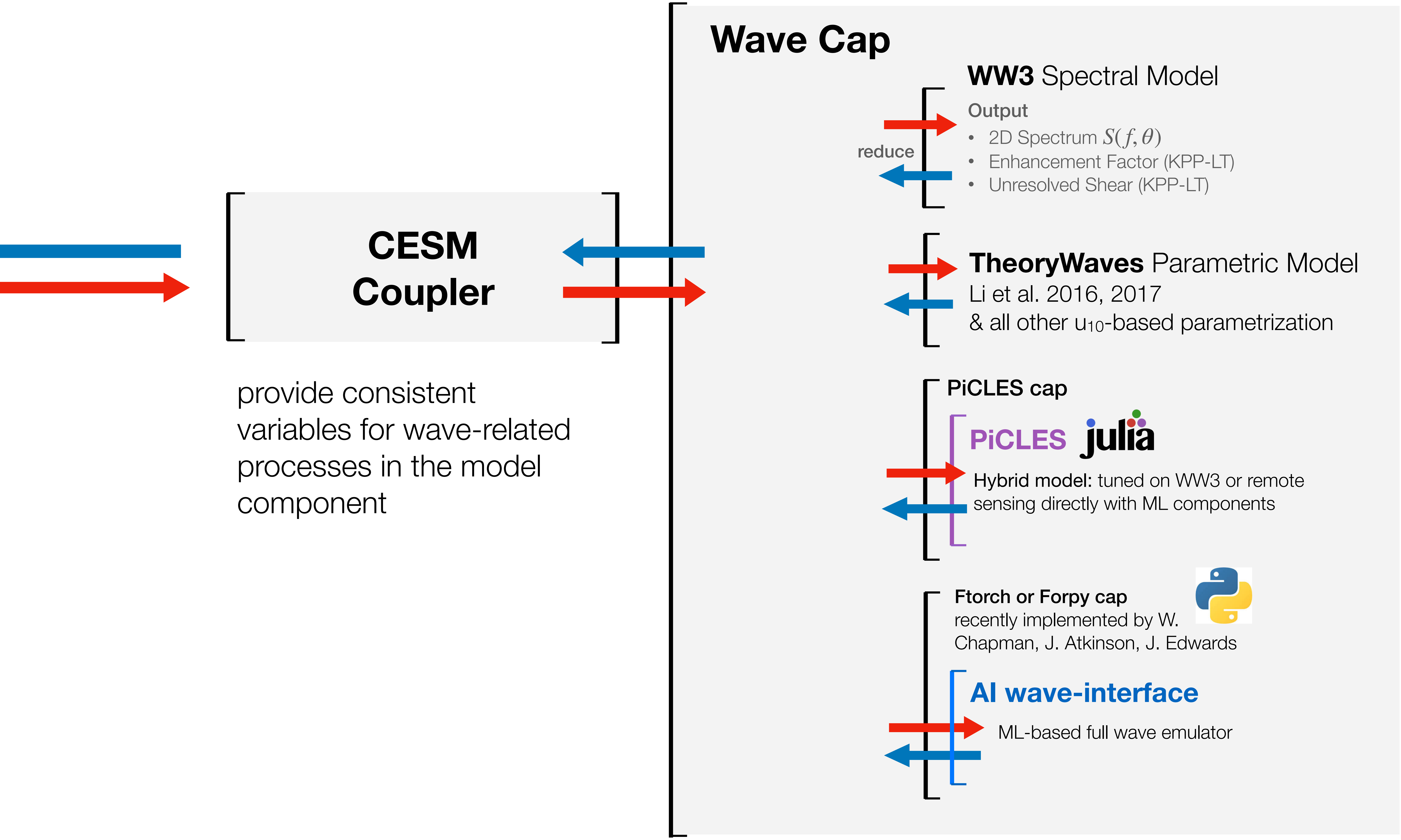
Enabling better physics and a basis for machine learning



Plan to improve the air-sea processes in CESM3

Implementing a standard, unified wave-coupling through NUOPC

Bill Sacks, Gerhard Theurich, Paul Hall



How to interface with Julia with a FORTRAN model structure

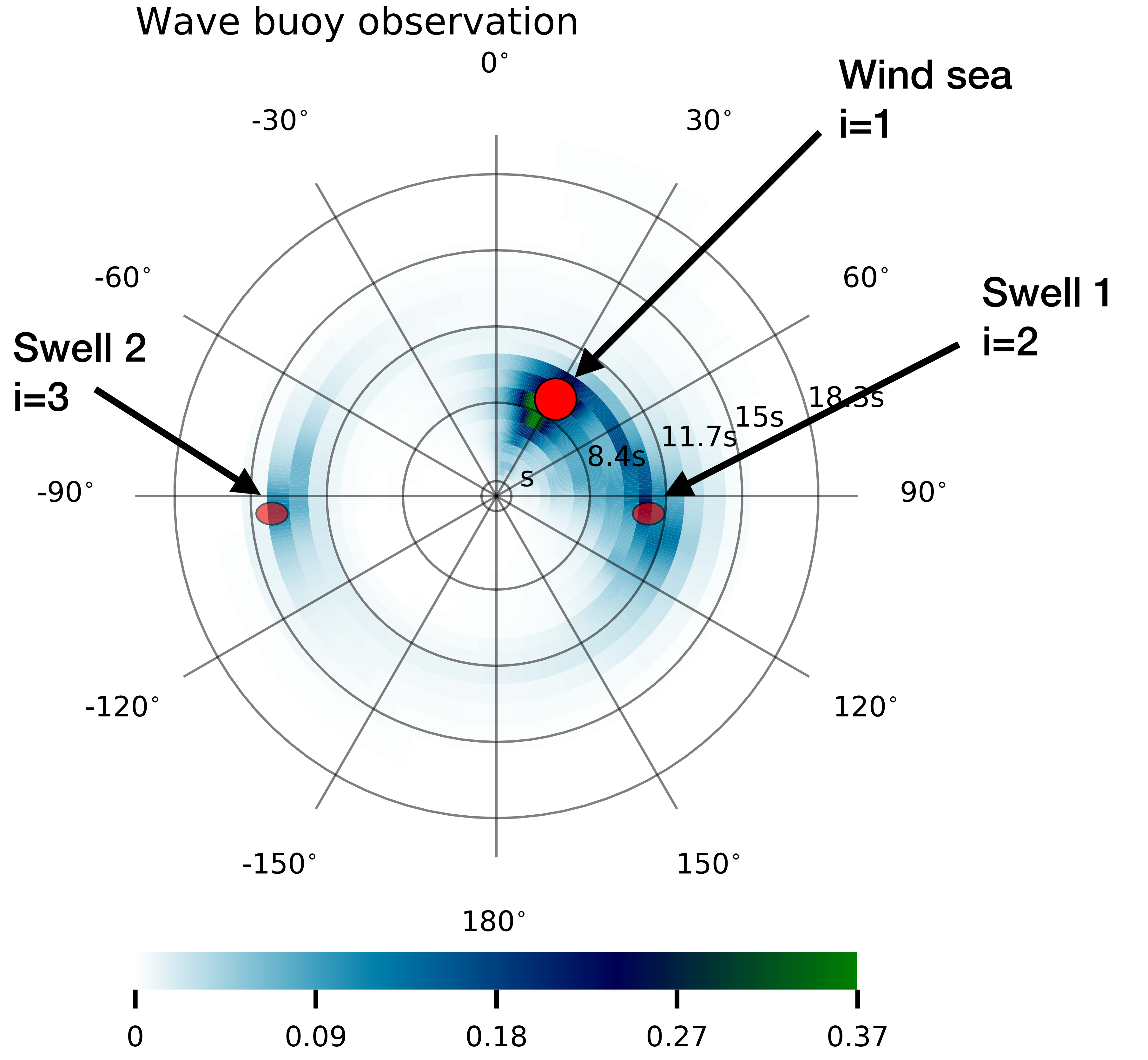
a) **FORTRAN-based NUOPC cap** that calls a FORTRAN <—> C <—> Julia interface

b) **C-based NUOPC cap** that then calls Julia interface

c) **Julia-based NUOPC cap** that is then native to PiCLES and other models

Moment based metrics for CIME/NUOPC-based wave-coupling

Baylor FK, Brandon Reichl, Paul Hall, Jessica Meixner, Adrian Webb, Qing Li



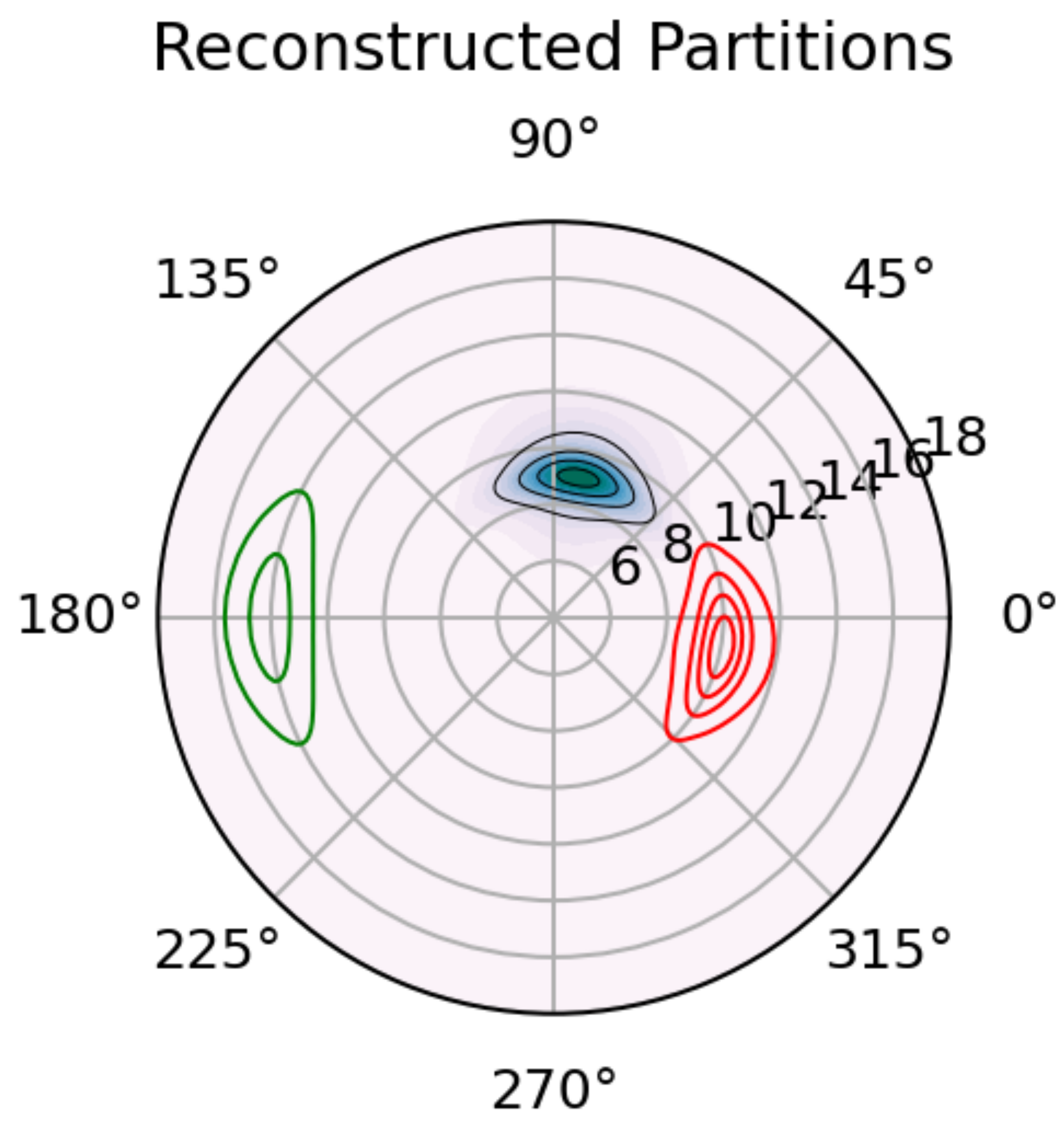
Output from *any* wave model

per wave system i (wave partition):

$$\begin{bmatrix} \vec{c}_{gp} \\ f_p \\ m_0 \\ m_1 \\ m_2 \\ z_0 \\ \vec{u}^s \end{bmatrix}_i$$

Vector of 9 x N partitions

Based on $[\vec{c}_{gp}, m_0]_i = [\theta, f_p, H_s]_i$



Standard wave bulk quantities with:

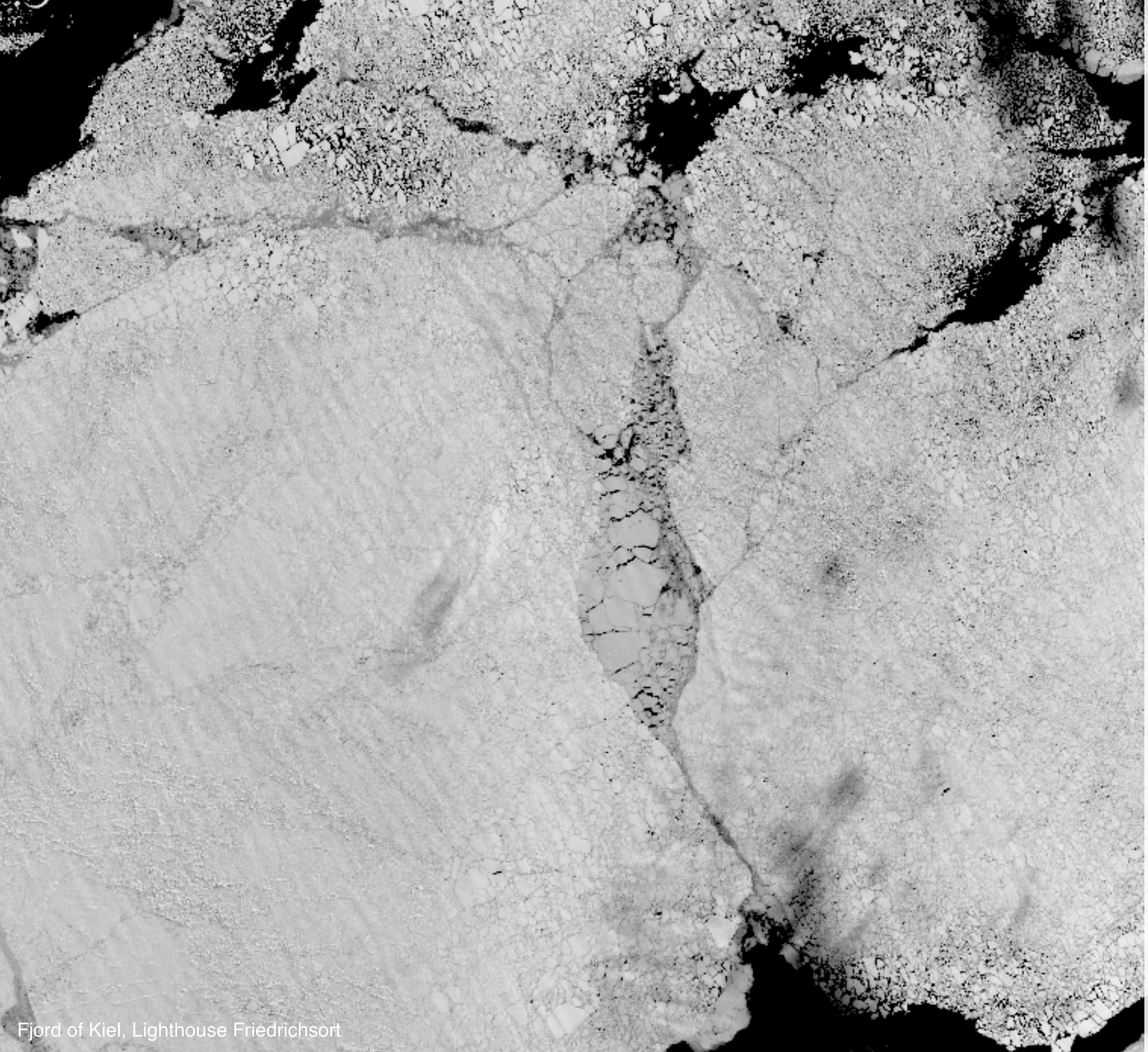
- **added tail approximation** for wind sea (i=0), Webb & FK 2011, 2015
- (maybe) **added attenuation factor** for high frequencies

Example processes:

Stokes Drift and ML-shear (m3, m1)

Sea spray (m1, m2)

Wave breaking (m4)



Fjord of Kiel, Lighthouse Friedrichsort

Thanks for you attendance

I am happy to take Questions