Particle-in-CelL for Efficient Swell *PiCLES*

Towards coupling with Earth System Models

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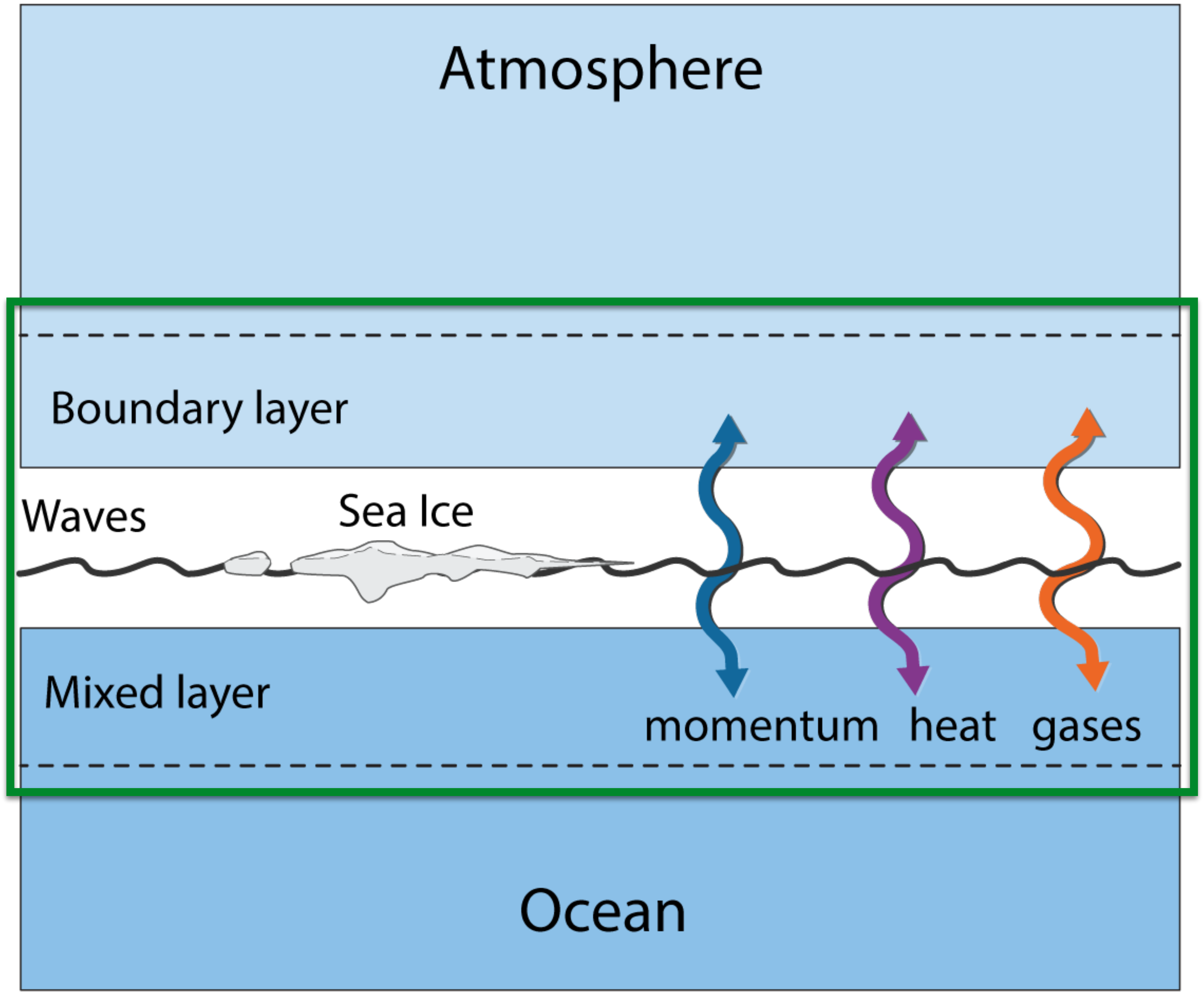
How do we model air-sea interaction in higher-resolution models?

We need to provide non-local, i.e. *not-equilibrated*
Waves in Earth System Model

Grid box of an earth system model



A framework for coupled boundary layers

Explicit, and efficient modeling of surface waves

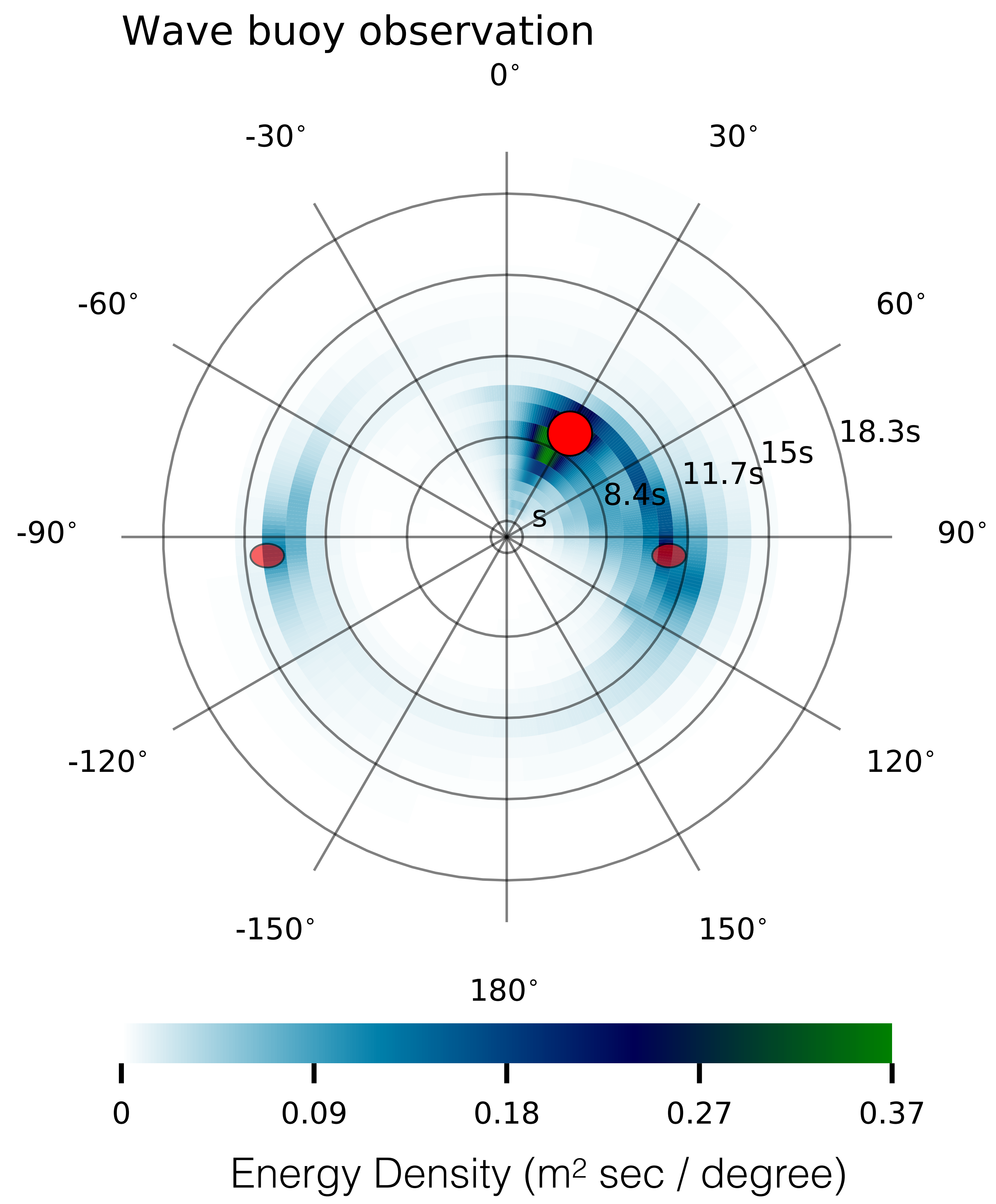
- better use remote-sensing data
- enable ML-based parametrization
- better represent processes at the interface

Why do we need waves in ESM today?

- Waves in the MIZ
- Stokes, Langmuir, and MLD
- White capping, sea spray, and gas fluxes
- Wave-current interaction (< 20 km)

Why can we not use a fully spectral wave model?

Directional wave spectra at Ocean Station Papa



Typical wave observations

- Wind sea & 1-3 Swell fields
- Each of these wave partition have **a direction, peak frequency, and energy**
- The total wave spectrum can be *approximated* by **9 variables**

Spectral wave model (WW3)

- discretize the wave action in frequency and direction
- needs **about 600 variables** to describe nearly the same information

Wave action equation

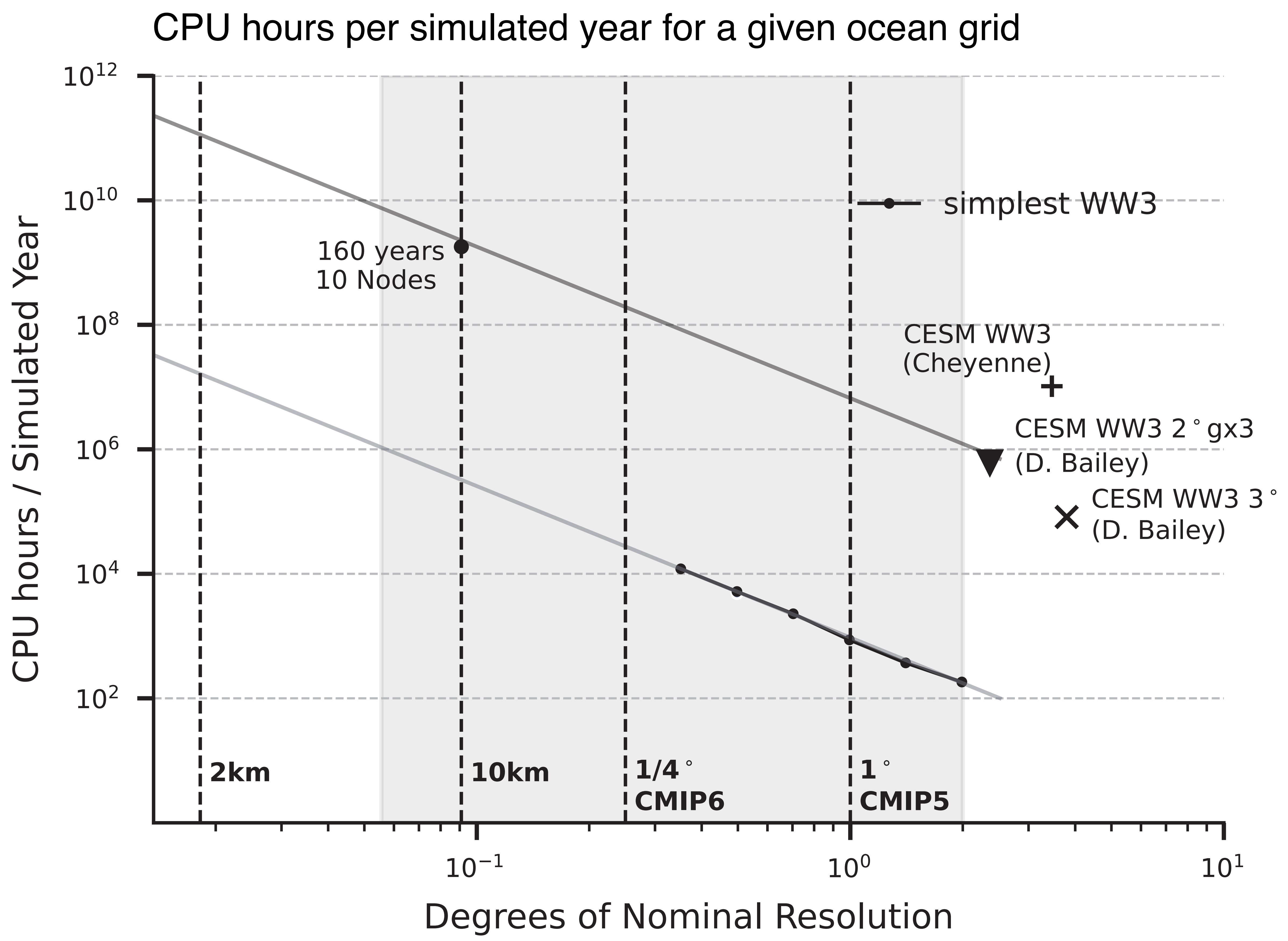
$$\frac{\partial}{\partial t} N + \nabla \cdot (c_g N) = S_{in} + S_{ds} + S_{nl}$$

$$N(x,\ y,\ t,\ k,\ l)$$

Spectral models are too expensive for global high-resolution integrations

Spectral Models in ESMs

- Large state vector (~600)
- coupling has likely large overhead
- S_{nl} is expensive
- WaveWatch III resolution in CESM is currently reduced to 3°



It would be good to understanding the bottlenecks of WW3 in CESM a little better!

2nd generation+ wave model

PiCLES

- Solves the wave field along Lagrangien trajectories (particles) that are re-meshed periodically
- Each particle is a representative sample for wave energy & momentum of wave system

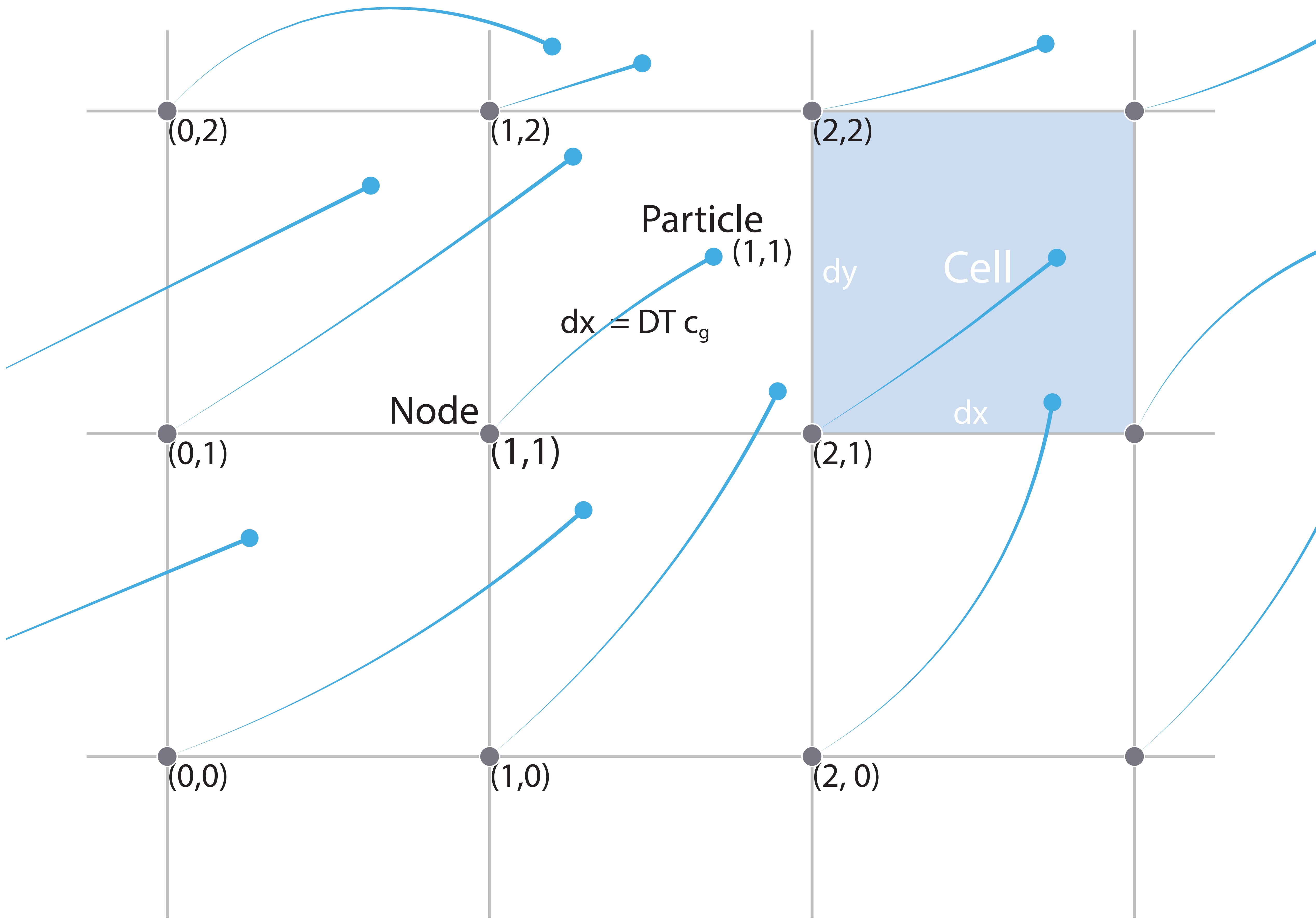
Main Objective:

Trade accuracy for speed and convenience!

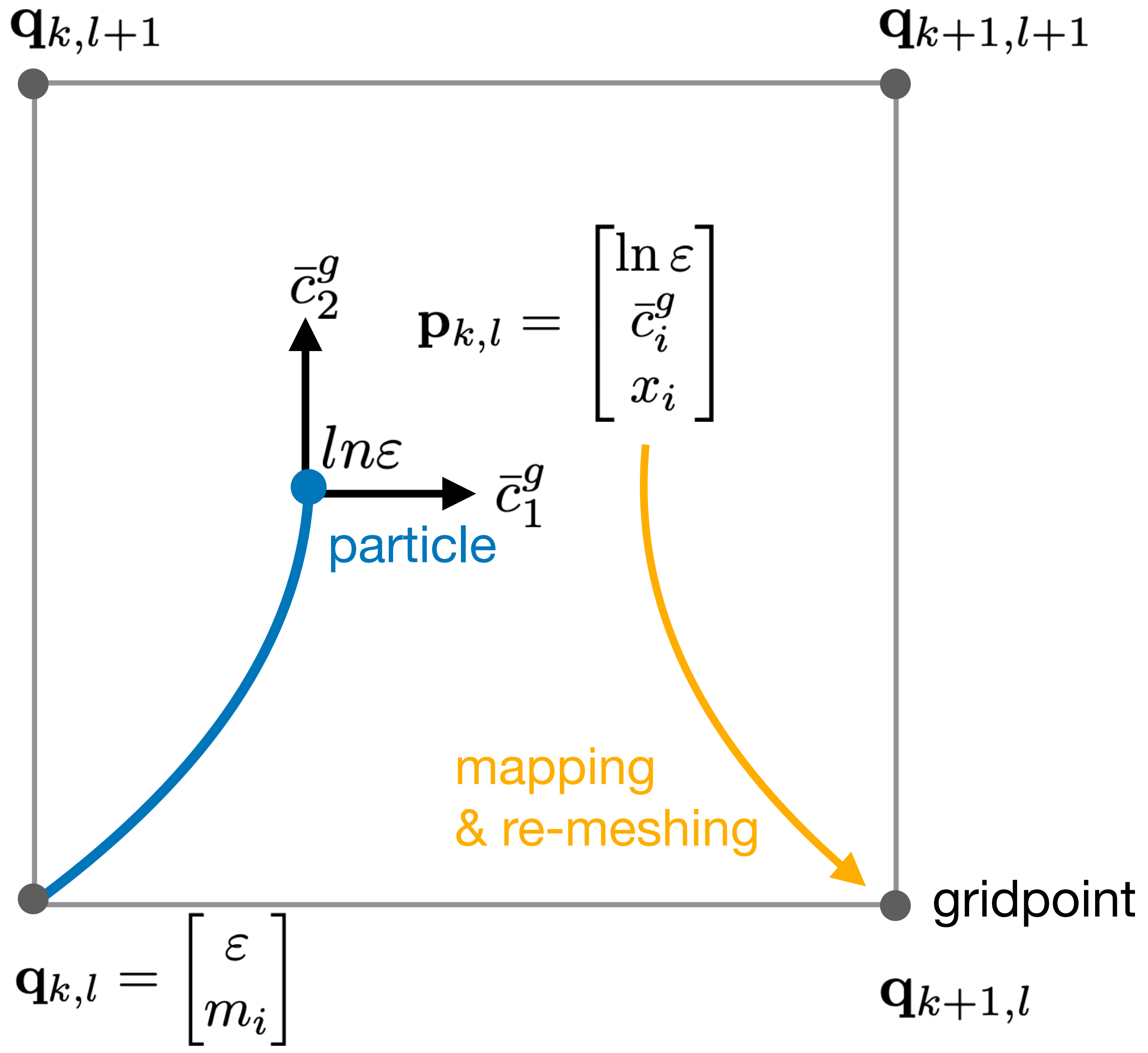
- Find alternative to reduce the high-dimensionality to **improve efficiency**
- Describe **sufficiently accurate** surface statistics for air-sea interaction in Earth System Models.

Key requirements

- Minimize particle interaction
- Designed to be parallel on GPUs
- Written in julia
- Focus on open-ocean waves



Equations to solve along a 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)

Then we can write down the **particle equations:**

parameterized wave-wave interaction

Similar to WW3

Particle Equations

$$\frac{d}{dt}ln\varepsilon = \quad \sigma_p\, r_g^2\, \tilde{S}^{cg} \quad + \sigma_p(\tilde{I} - \tilde{D}),$$

$$\frac{d}{dt}\bar{c}^g_i = -\bar{c}^g_i\; \sigma_p\, r_g^2\, \tilde{S}^{cg} + [\bar{c}^g_2, -\bar{c}^g_1]^T\; \sigma_p\; \tilde{S}^{dir}$$

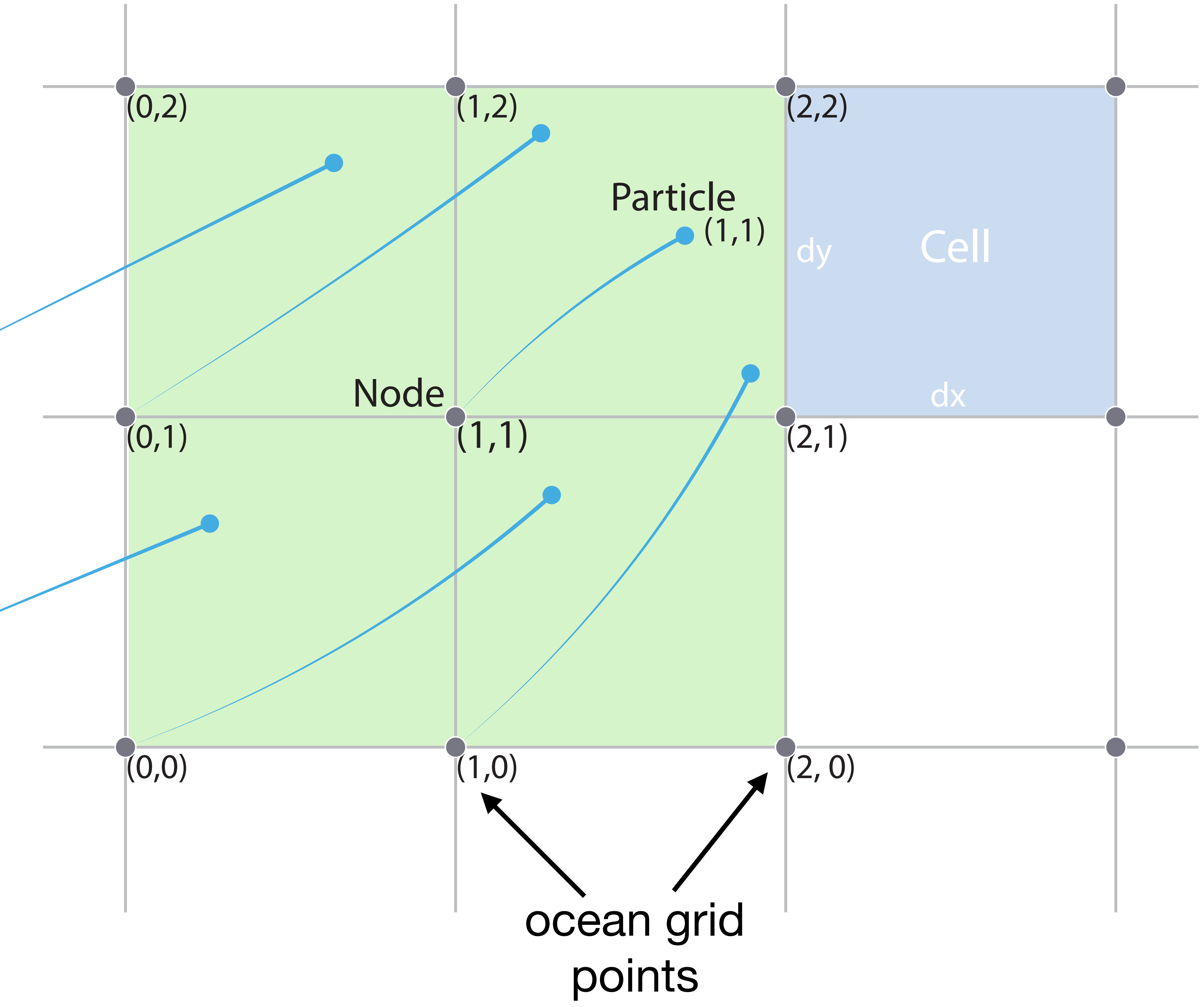
$$\frac{d}{dt}x_i = \bar{c}^g_i.$$

Parametrized change in direction

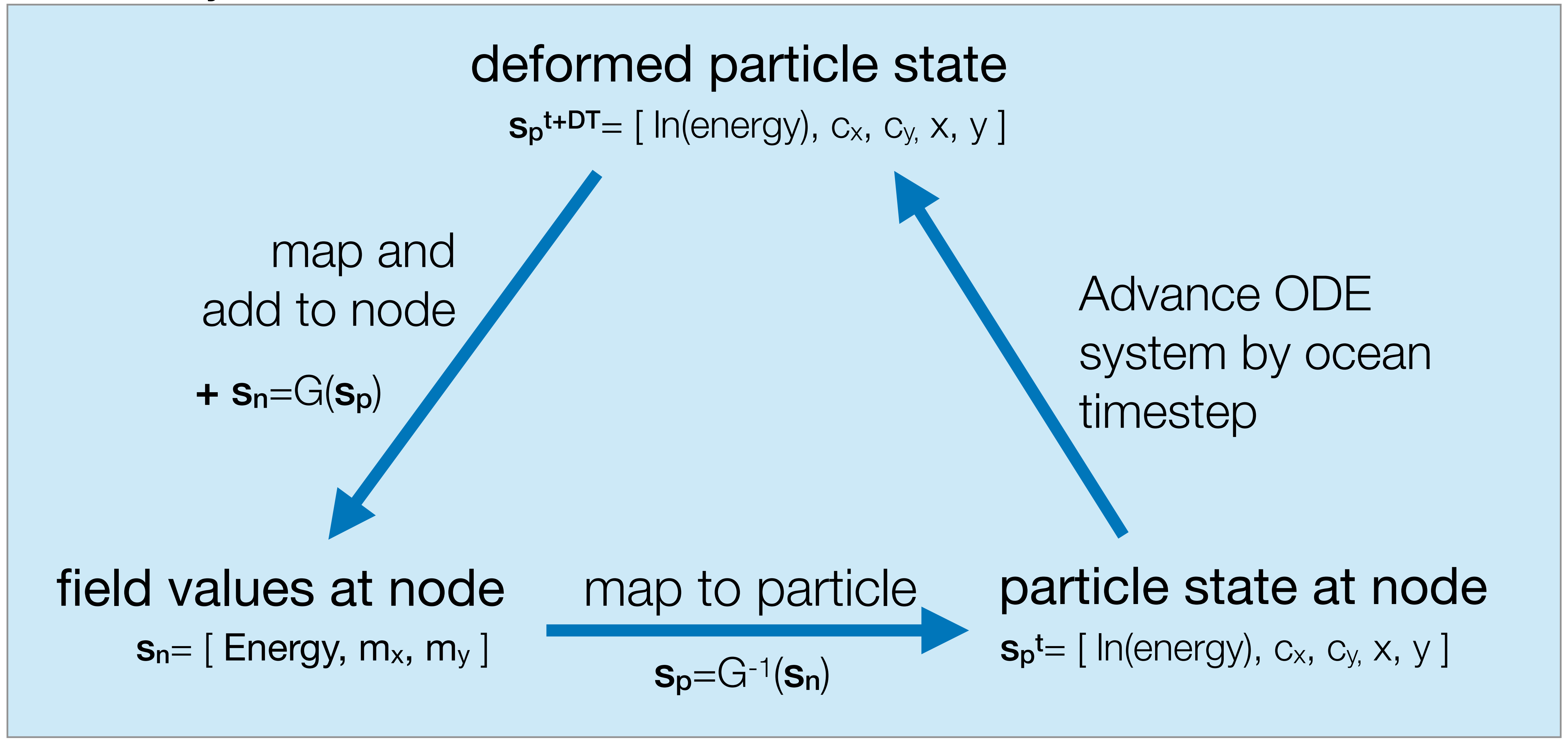
- Wave-wave interaction along the trajectory is parametrized
- Wave-wave interaction normal to the particle trajectory are often small and modeled in the re-meshing step

Advance and re-mesh

Lagrangian wave growth + Particle-in-Cell = PiCLES



Model cycle



$$\hat{\boldsymbol{m}} = \sum_n^N w_n \boldsymbol{m}_n,$$

- re-meshing conserves energy and momentum

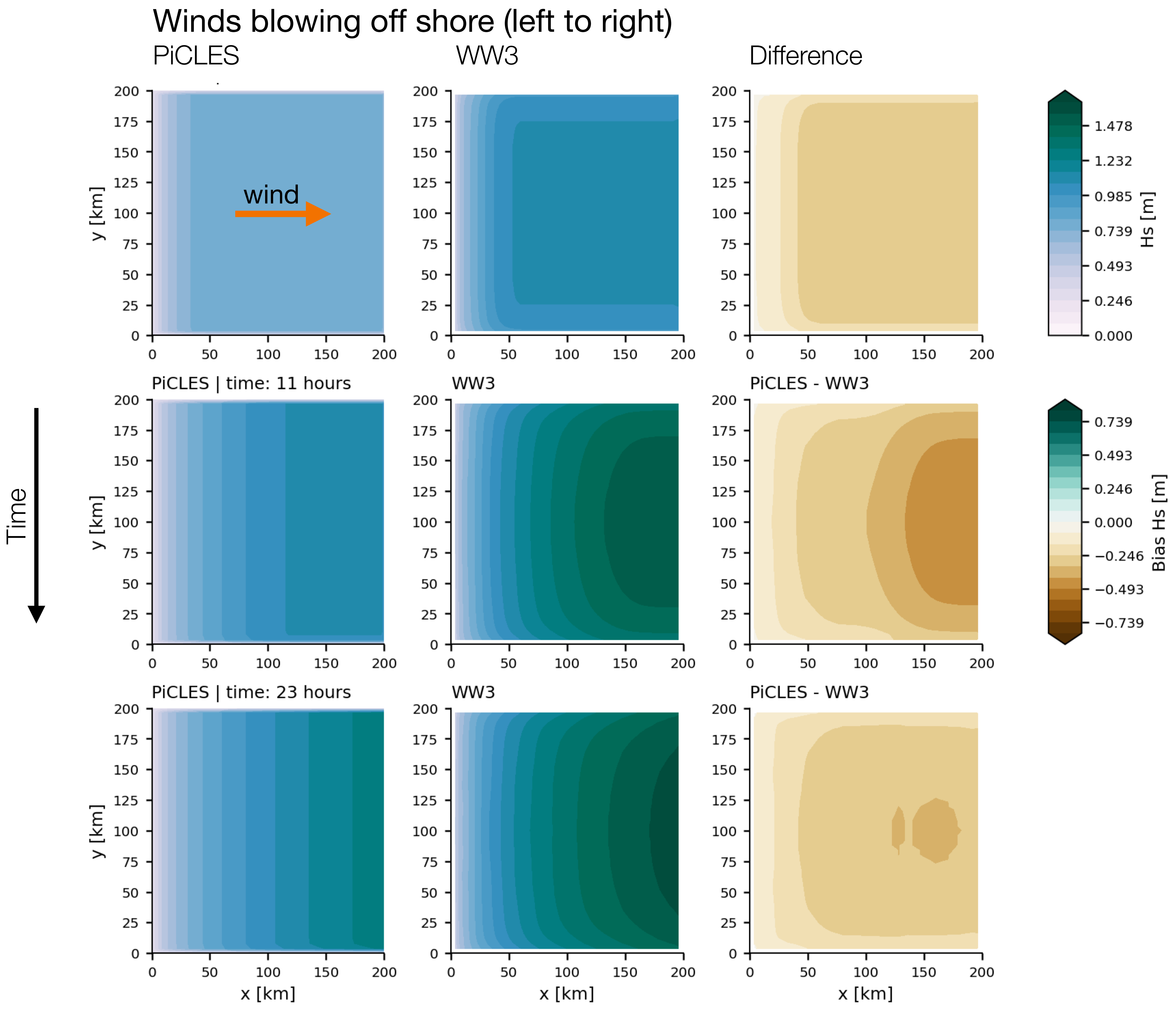
$$\hat{e} = \sum_n^N w_n e_n,$$

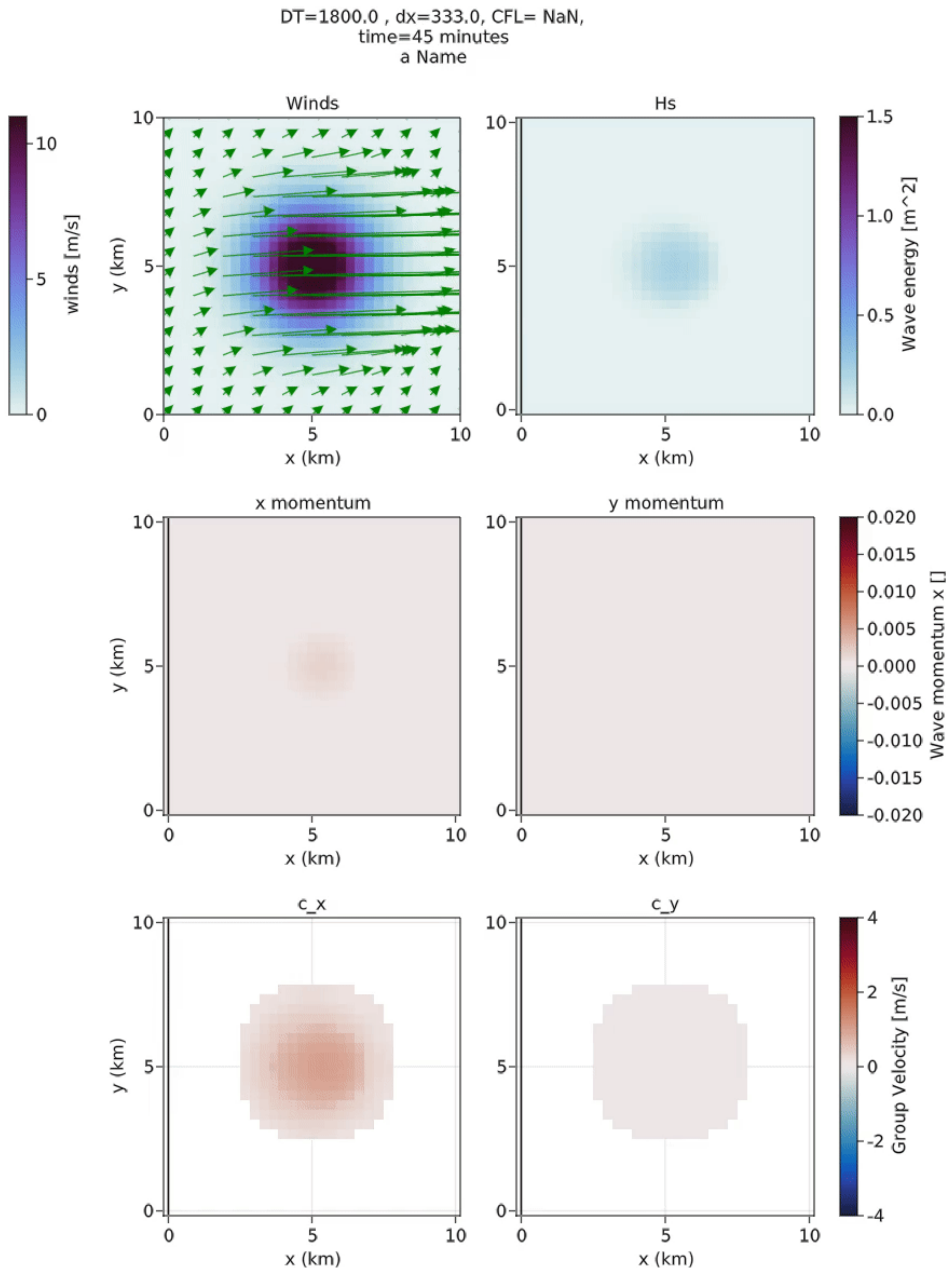
Particle-In-Cell weights

Accuracy: Comparing to WW3

The general model structure works well, but

- dispersion and diffusion not yet implemented
- amplitudes are not tuning yet. We will use **Ensemble Kalman Sampling**



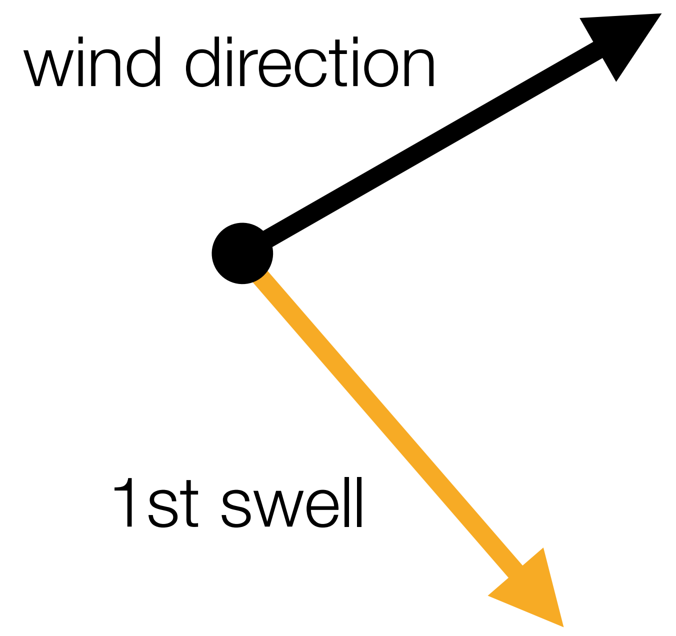


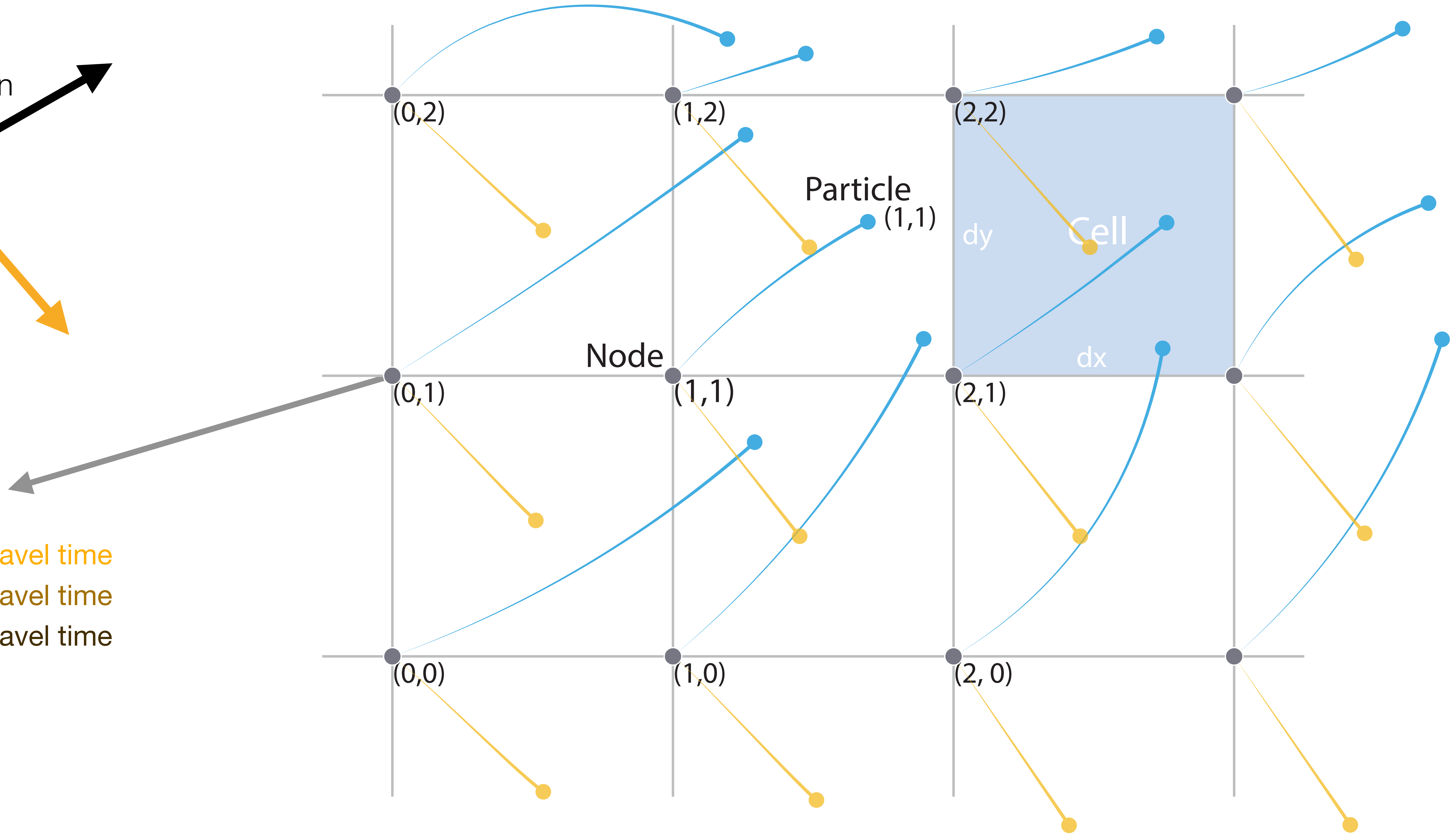
Example

Time-varying wind sea

Propagating swell

How? We take the model x 4!





Each node has multiple particles

Wind sea: 1 x 5 **energy, cg_x, cg_y, x, y**

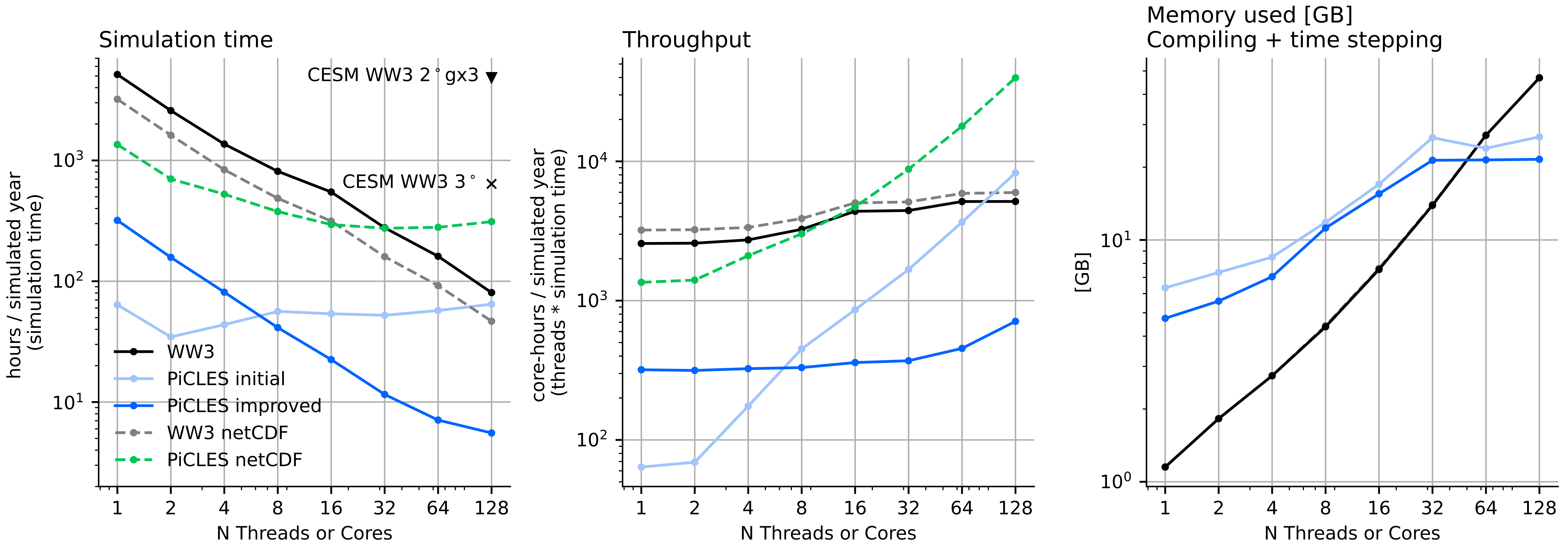
Swell I: 1 x 5 energy, cg_x, cg_y, x, y, + age or travel time

Swell II: 1 x 5 energy, cg_x, cg_y, x, y, + age or travel time

Swell III: 1 x 5 energy, cg_x, cg_y, x, y, + age or travel time

Strong Scaling Test

Sub-optimal PiCLES might be sufficient



Strong scaling for $\approx 0.7^{\circ}$ $(N = 512^2)$ on 1 derecho Node

PiCLES

- Currently only multithreading
- about 10x faster,
- 3-4x more allocating, but less throughput

WW3

- openMPI
- Scales, and allocated well for the size of the state vector.
- about 120x more variables.

Weak Scaling Tests - Out-running WW3

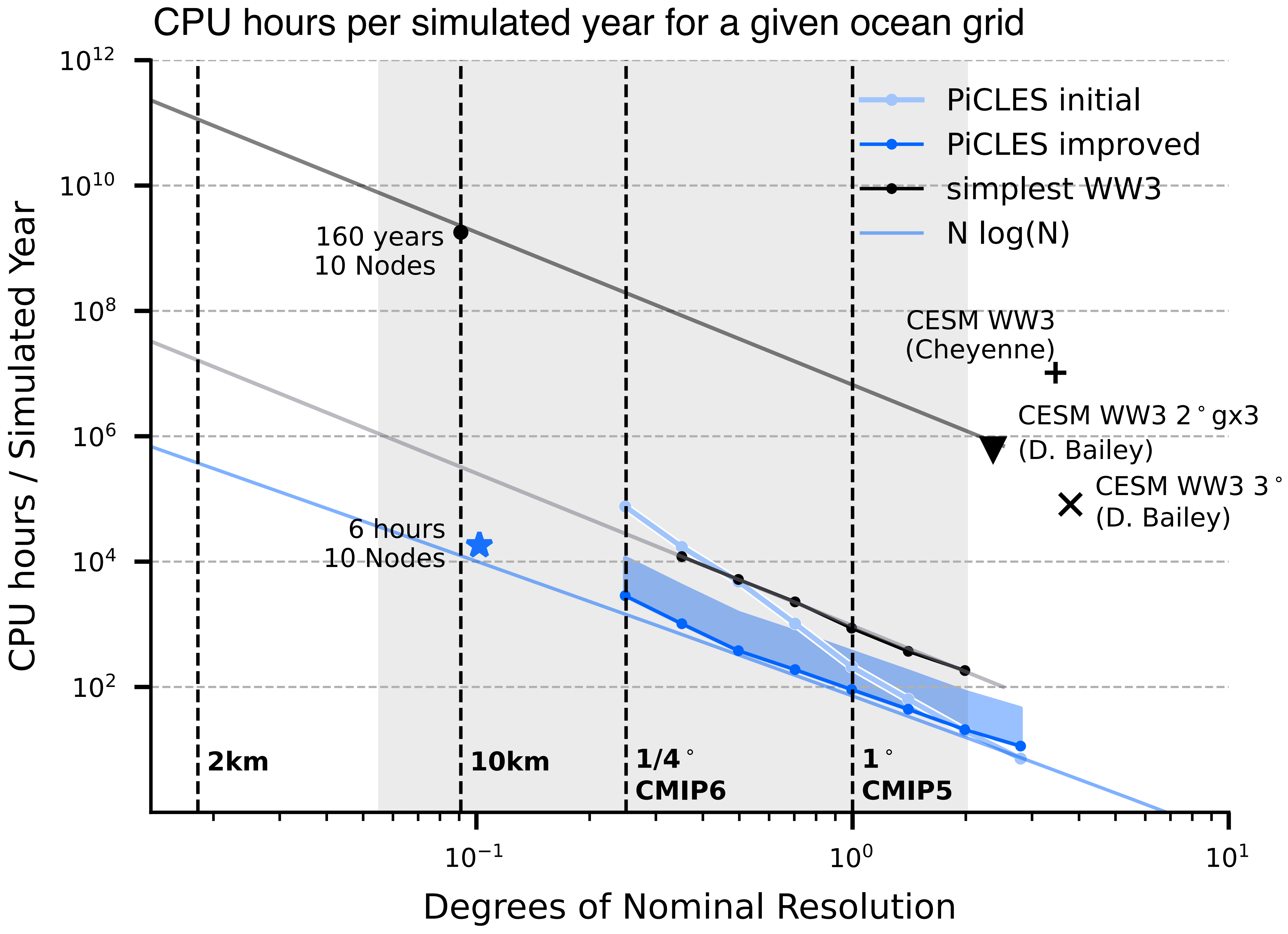
A semi-interactive wave model is **substantially more efficient** for future Earth System Models

Spectral Models in ESMs

- Large state vector (~600)
- coupling has likely large overhead
- S_{nl} is expensive
- WaveWatch III resolution in CESM is currently reduced to 3°

PiCLES:

- small state vector (about 5 - 20, depending on complexity)
- runs on the ocean grid and time step (no strict CFL condition)
- can be well optimized for GPUs
- for CMIP6-class models, we expect it at least run about an order of magnitude faster then WW3



- *current* PiCLES is $\mathcal{O}(10)$ faster then **WW3** ***without overhead*** and coupling
- PiCLES is about $\mathcal{O}(10^4)$ faster then **WW3** ***with overhead*** and coupling
- Once allocation is optimized, we expect PiCLES to scale better than N log(N)
- ★ We can already run wind-sea simulation on 10km resolution on 1 Node

It would be good to understanding the bottlenecks of WW3 in CESM a little better!

Implementation into CESM

Fortran/C coupler for Julia

- Thanks to Bill Sacks and Gerhard Theurich we have a minimal working example for Fortran -> C -> Julia
- We work on getting internal funding (NCAR) to develop a Julia (PiCLES) <-> fortran (NuOPC-CAP)

Cap & Coupling with CESM

- Unify implementation of wave-model in CESM
- see Paul Hall presentation and wave-cap discussion later in this session

Steps towards a stand-alone wave model

Challenges

1) Determine time stepping limits
2) Tuning/benchmarking
3) Emulating dispersion, diffusion, and refraction
4) Multi-layer & Merging rules
5) Optimize allocations

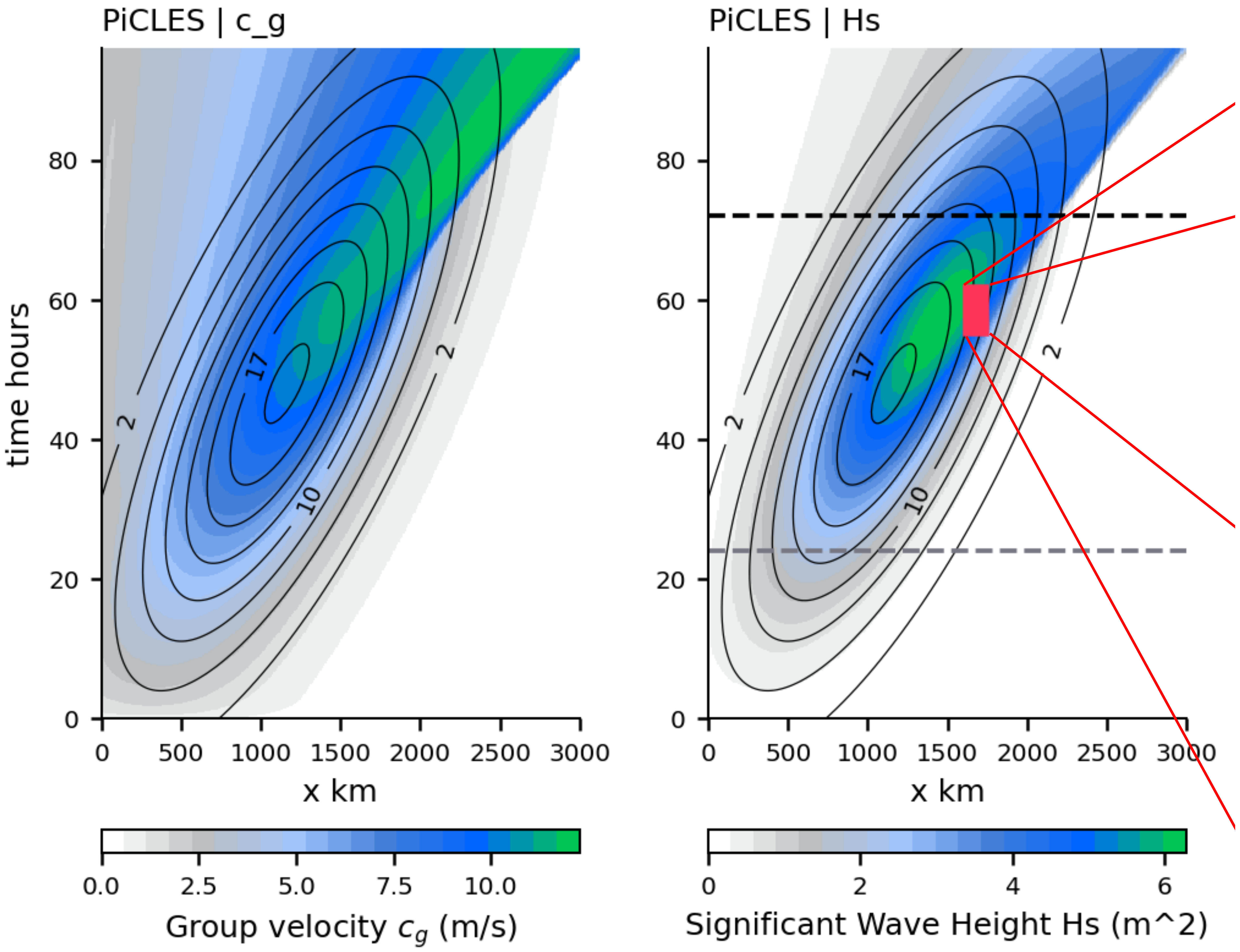
Stochastic wave-current interaction

PhD project of Tom Protin at Ifremer

(co-mentoring with Valentin Resseguier, Bertrand Chapron, and Ronan Fablet)

Test of wave growth under time-varying Forcing

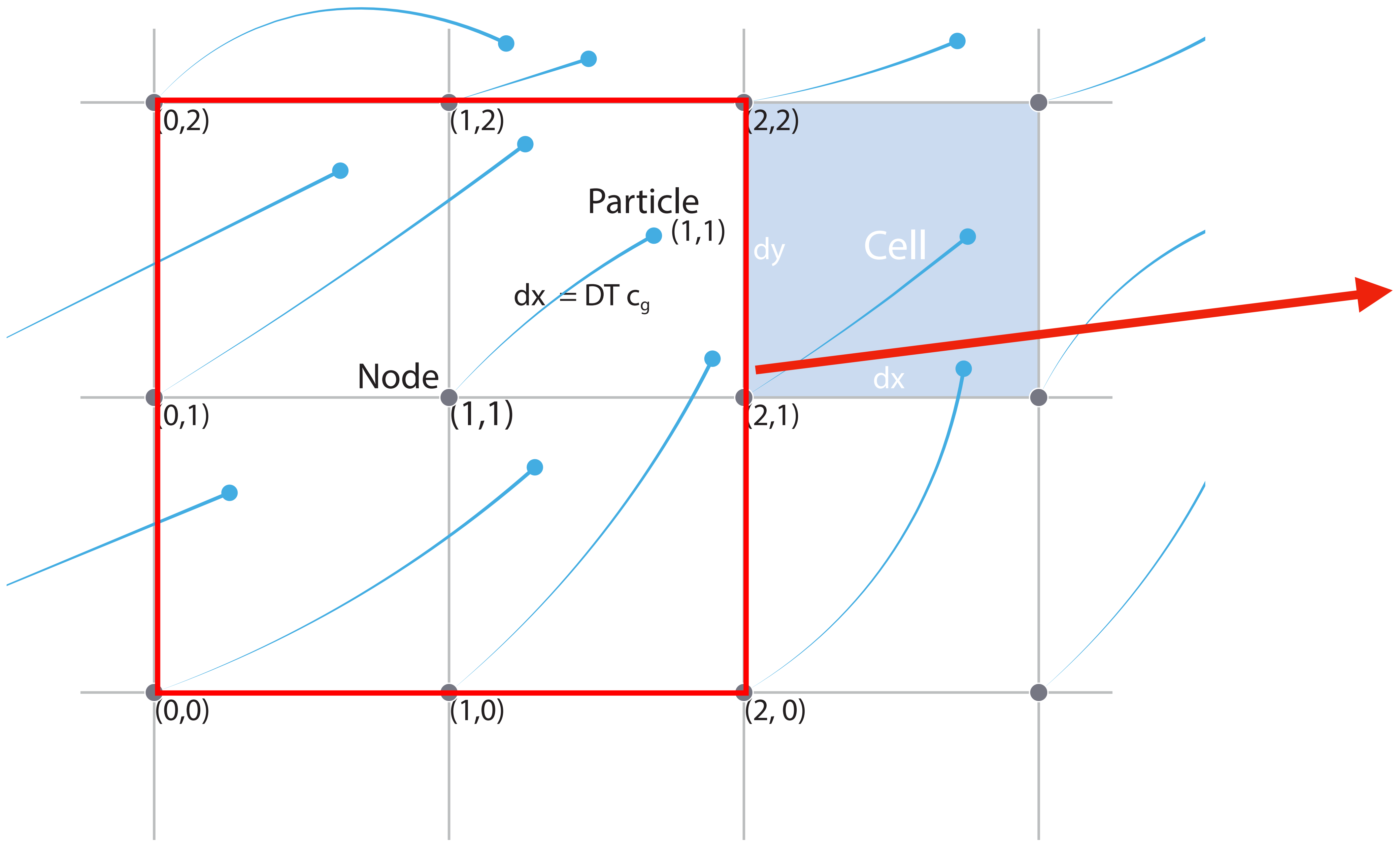
Growing waves in 1D

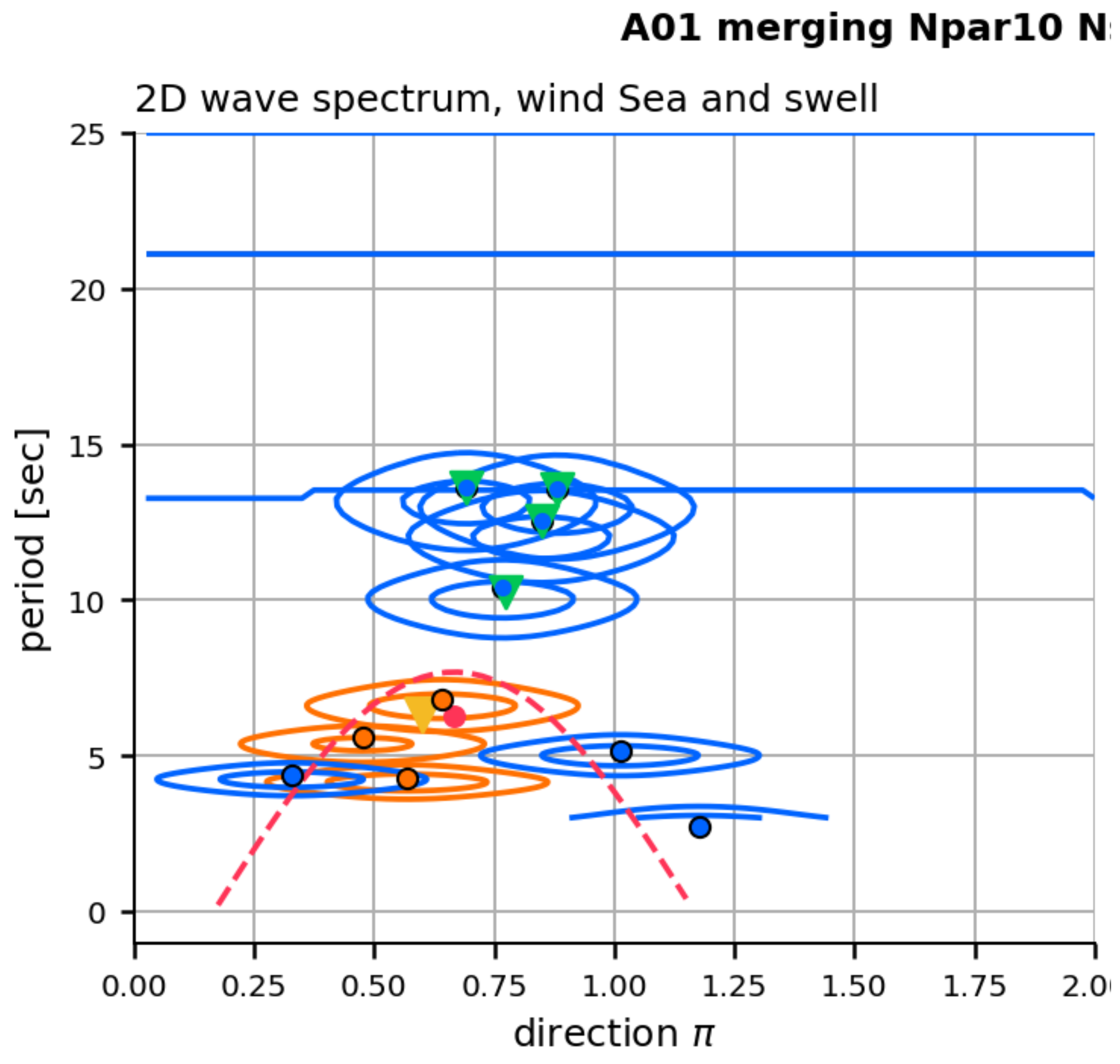


Qualitatively reproduces Hell et al 2021:

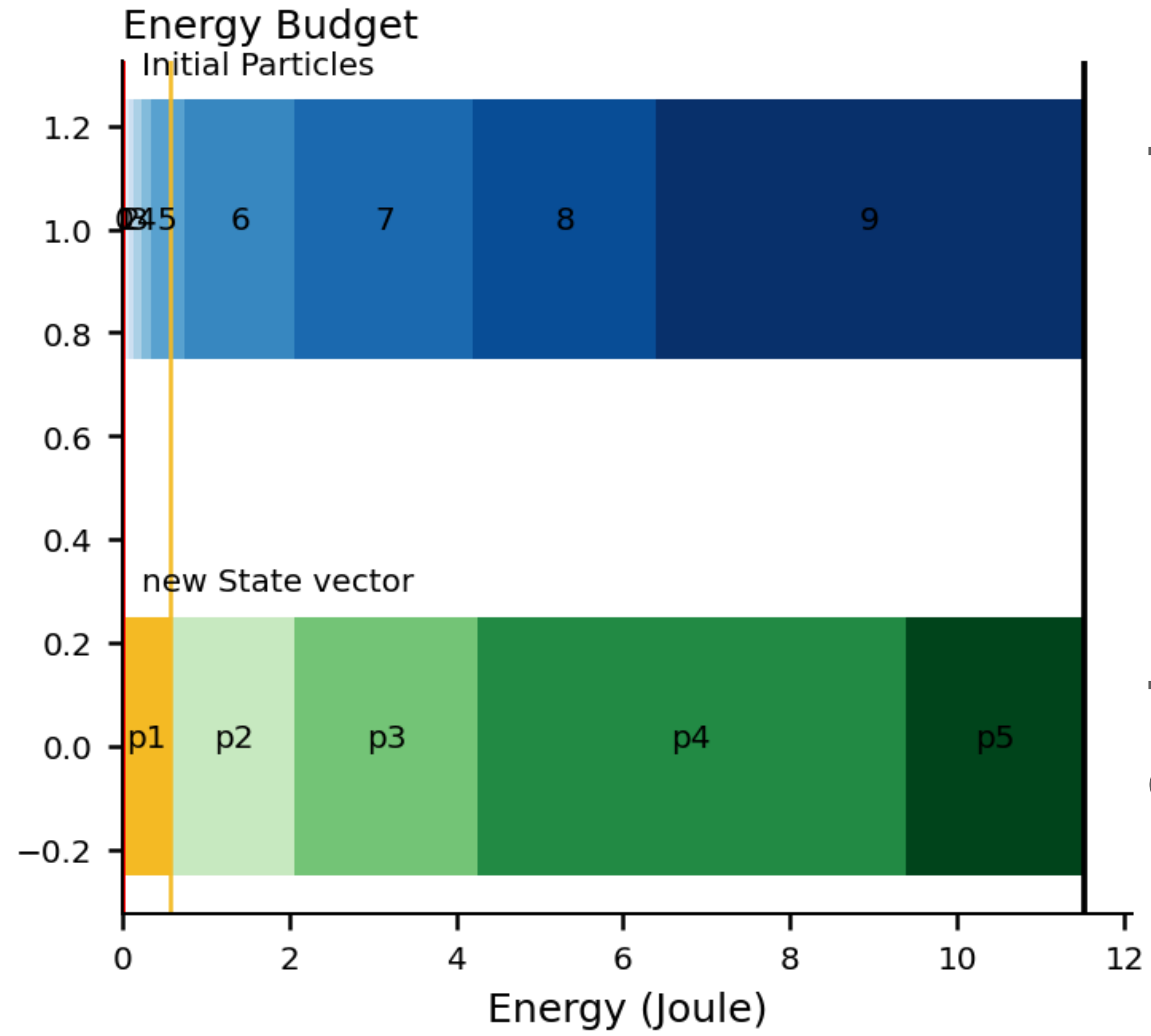
- highest wave speeds and energy ahead of the high-test wind speeds
- non-local effects under wave-growth conditions

Problem III: how to merge and how to separate between swell and wind sea?





- Merging/re-gridding should conserve energy and momentum, but on the same time not double count energy.
- wave growth is the result of the (5%) residual of wind energy input and dissipation



Total advected energy in proximity of the Node

Total re-initialized energy at the Node

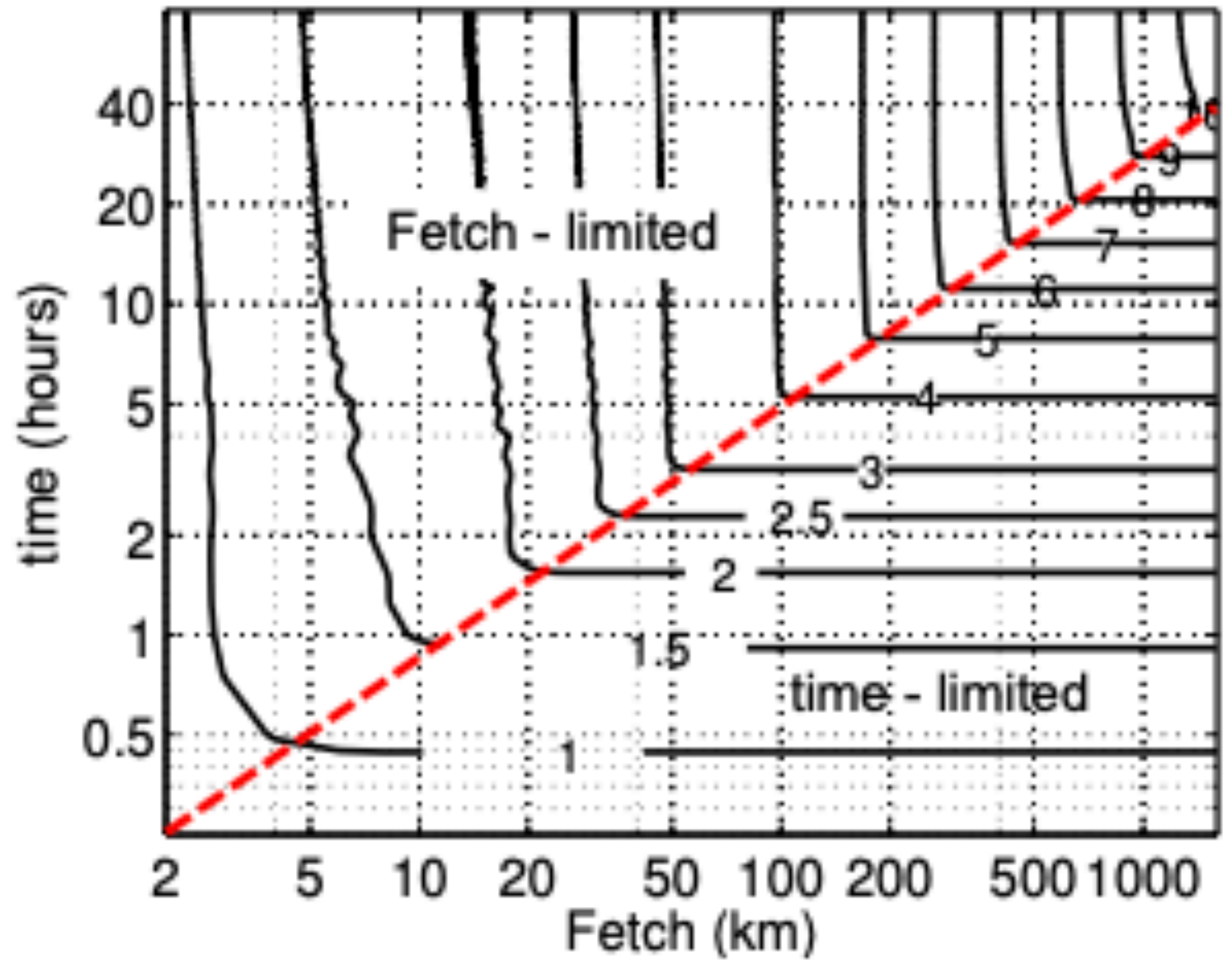
Test Case I: Static Fetch

Reproducing 2nd generation models

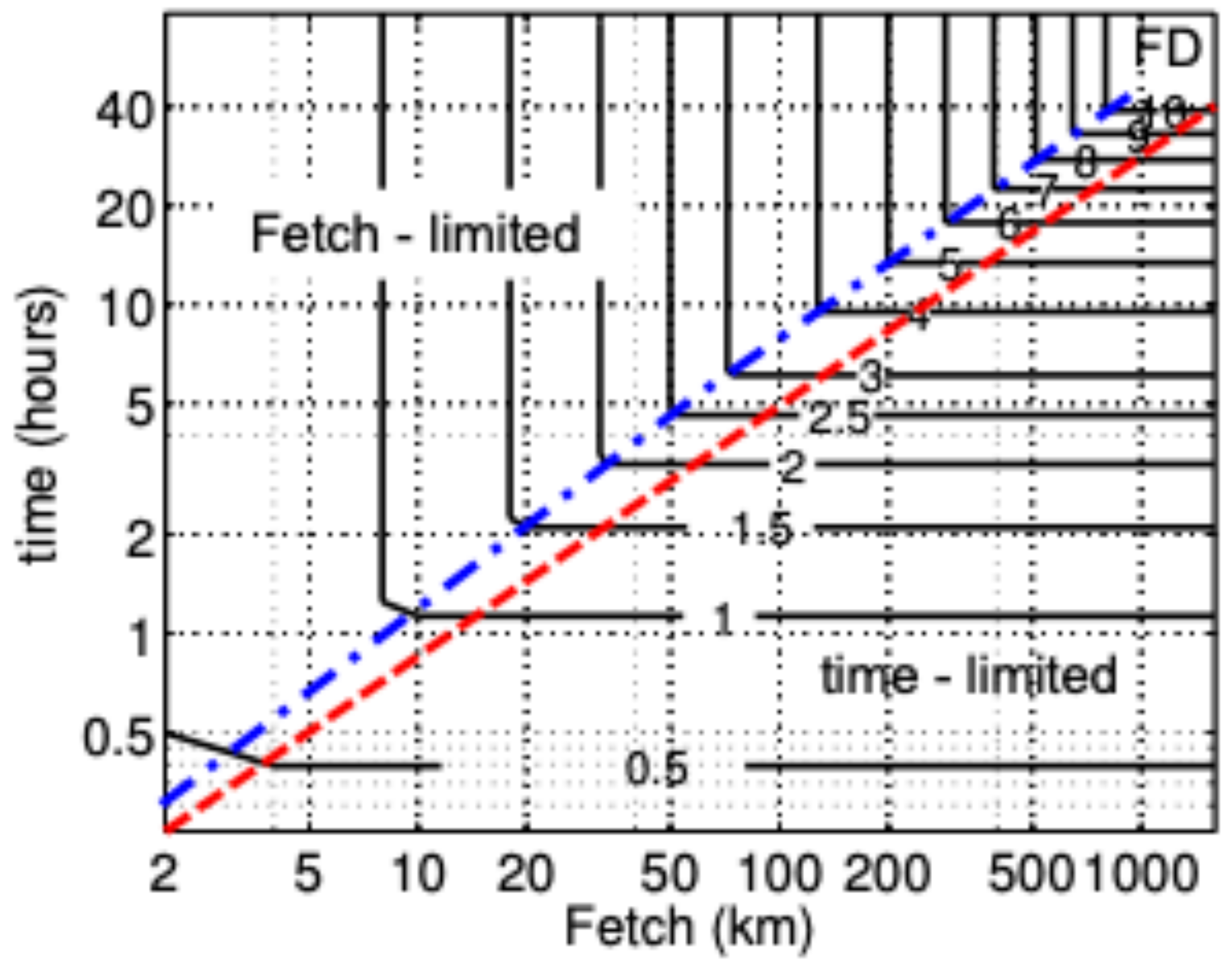
The model qualitatively reproduces the fetch relation well

- Numerical diffusion needs tuning of wave growth and dissipation
- We plan to calibrate using Ensemble Kalman Inversion (*Calibrate, Emulate, Sample*, Cleary et al. 2020)

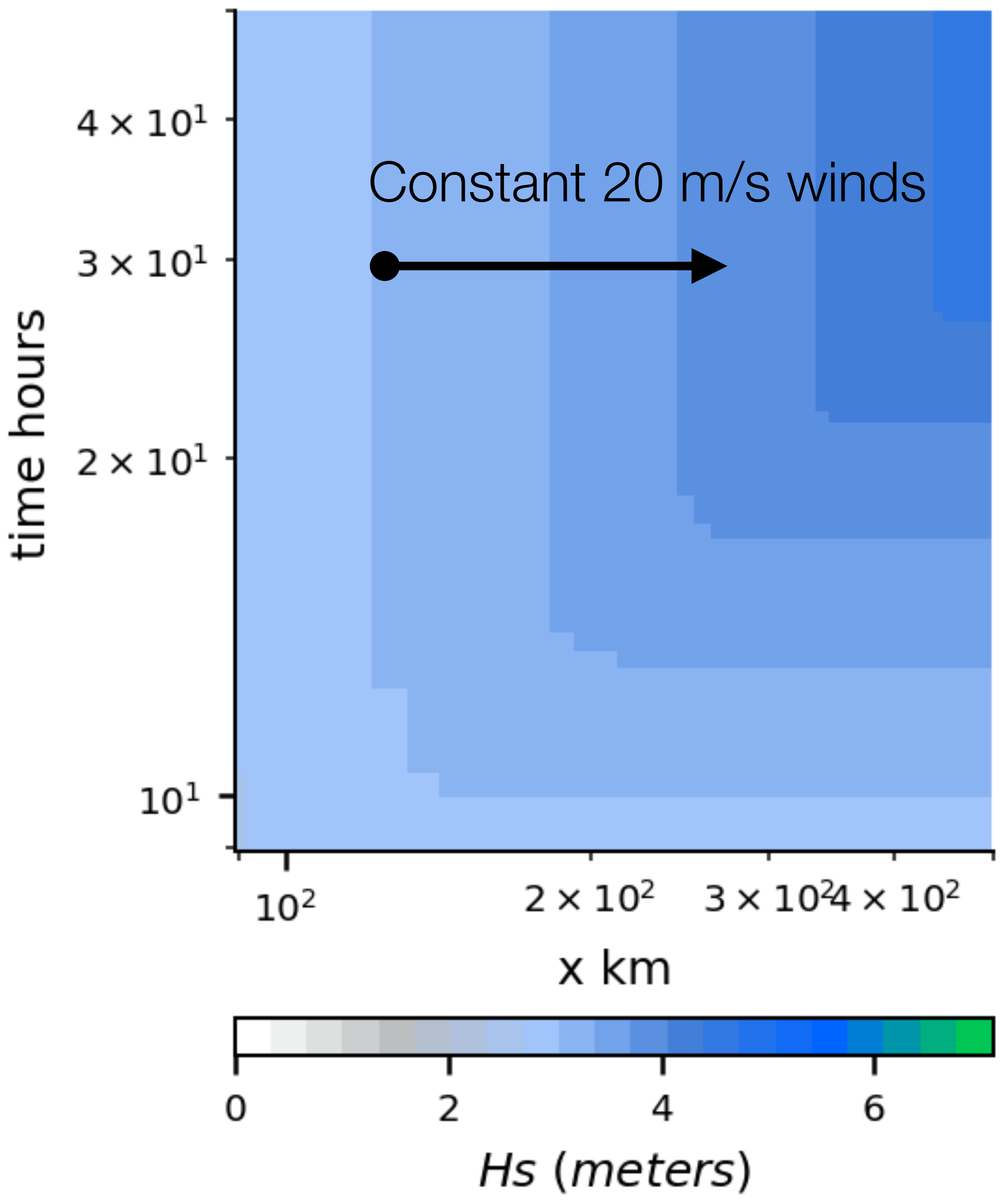
Wave Watch III test

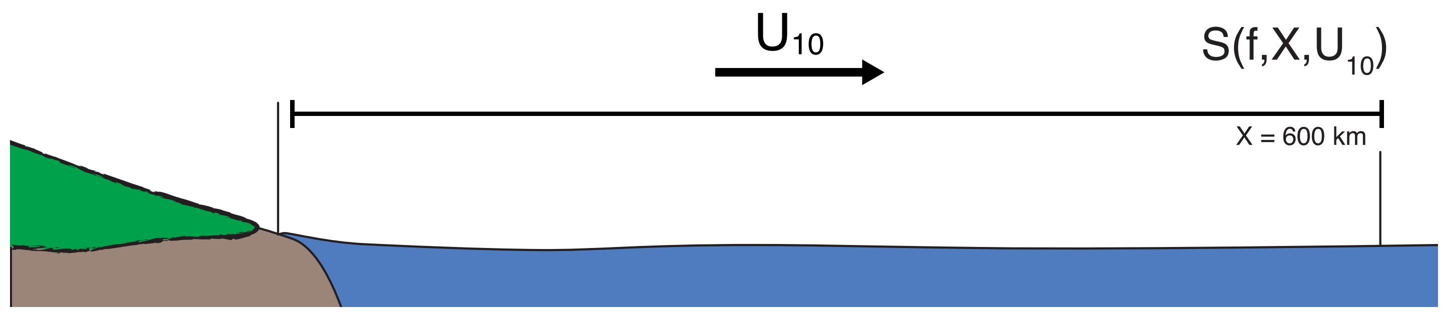


Static fetch laws (from F. Ardhuin's Book)



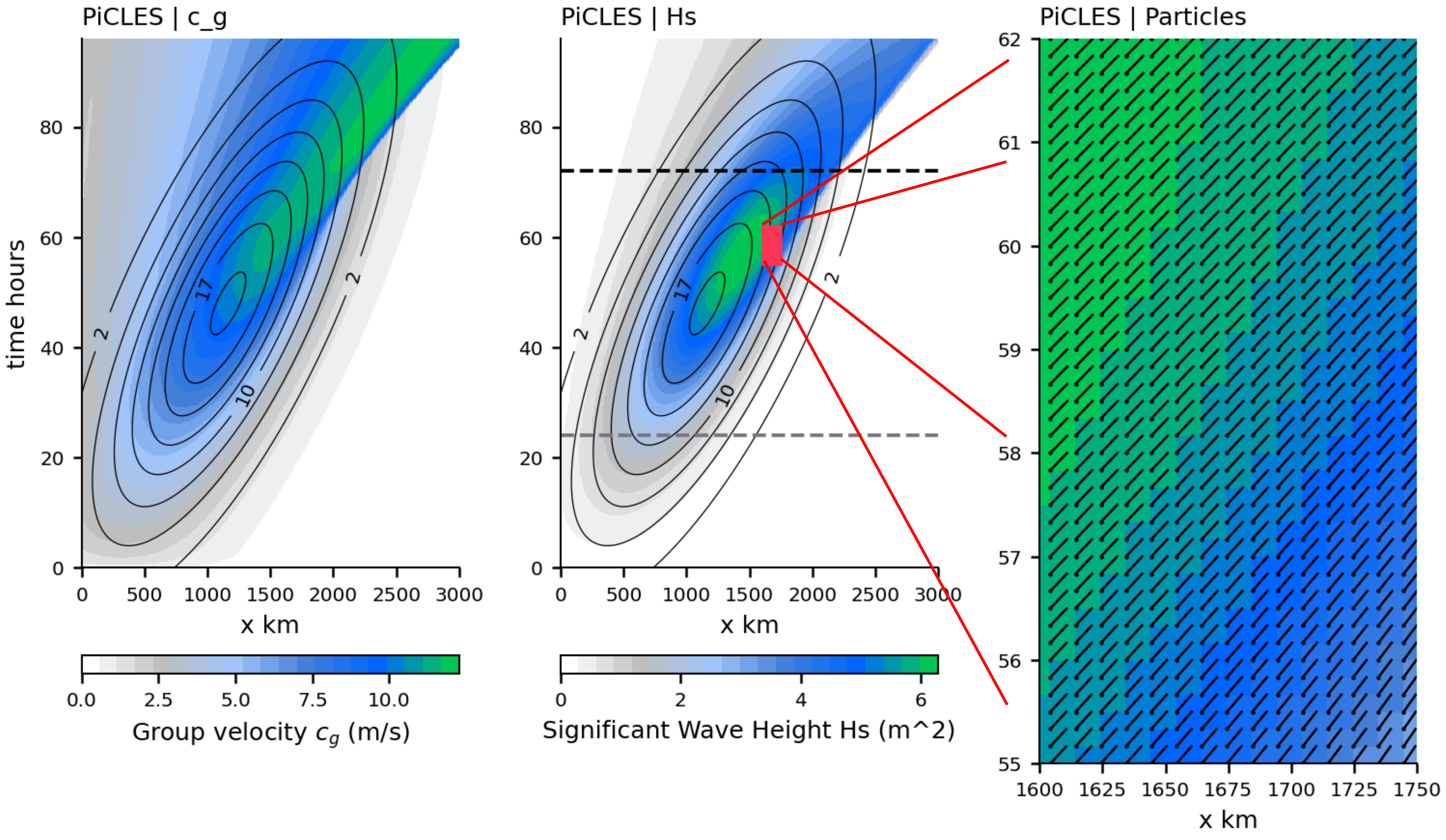
PiCLES model





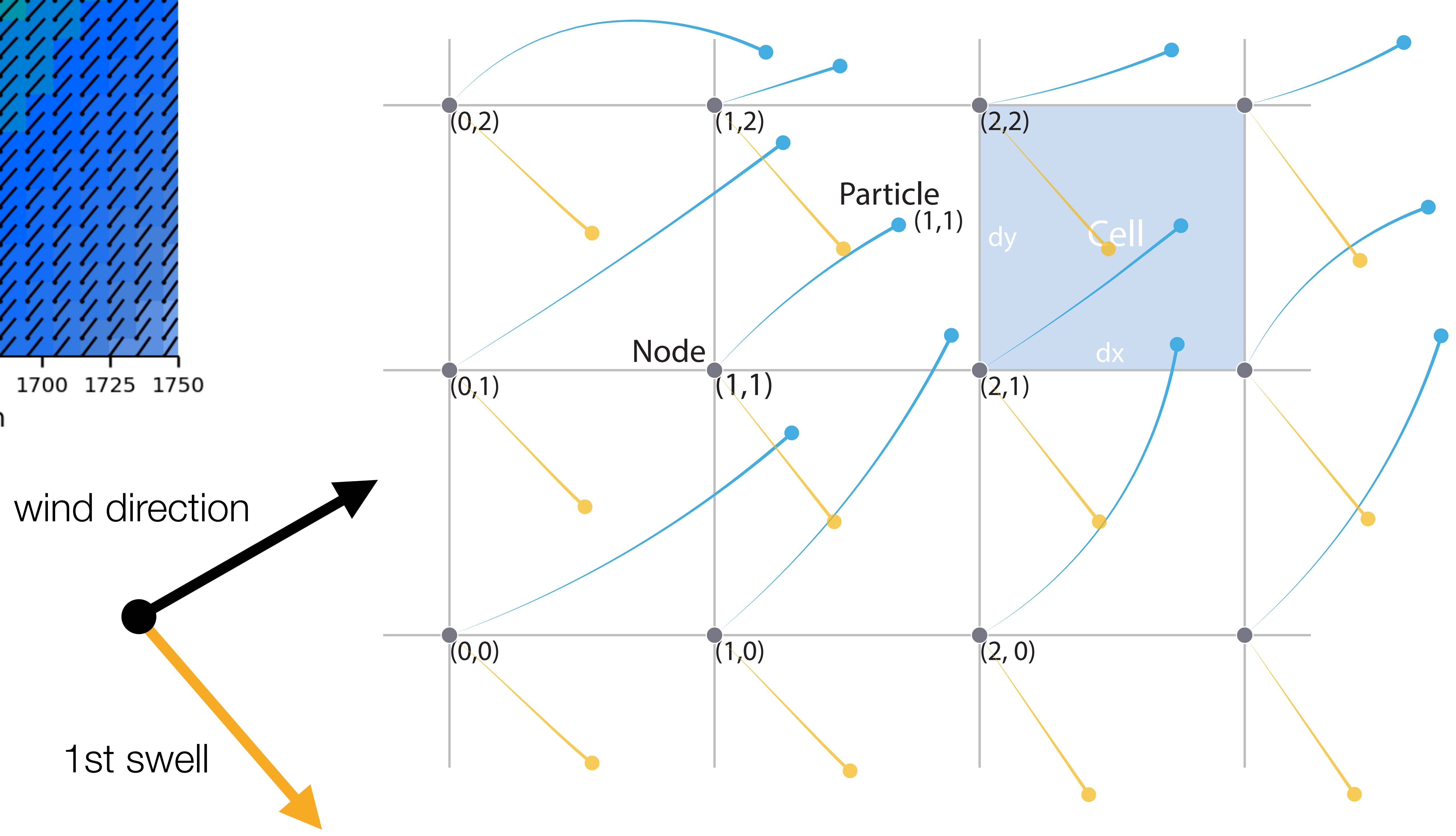
PiCLES: Dynamic Fetch

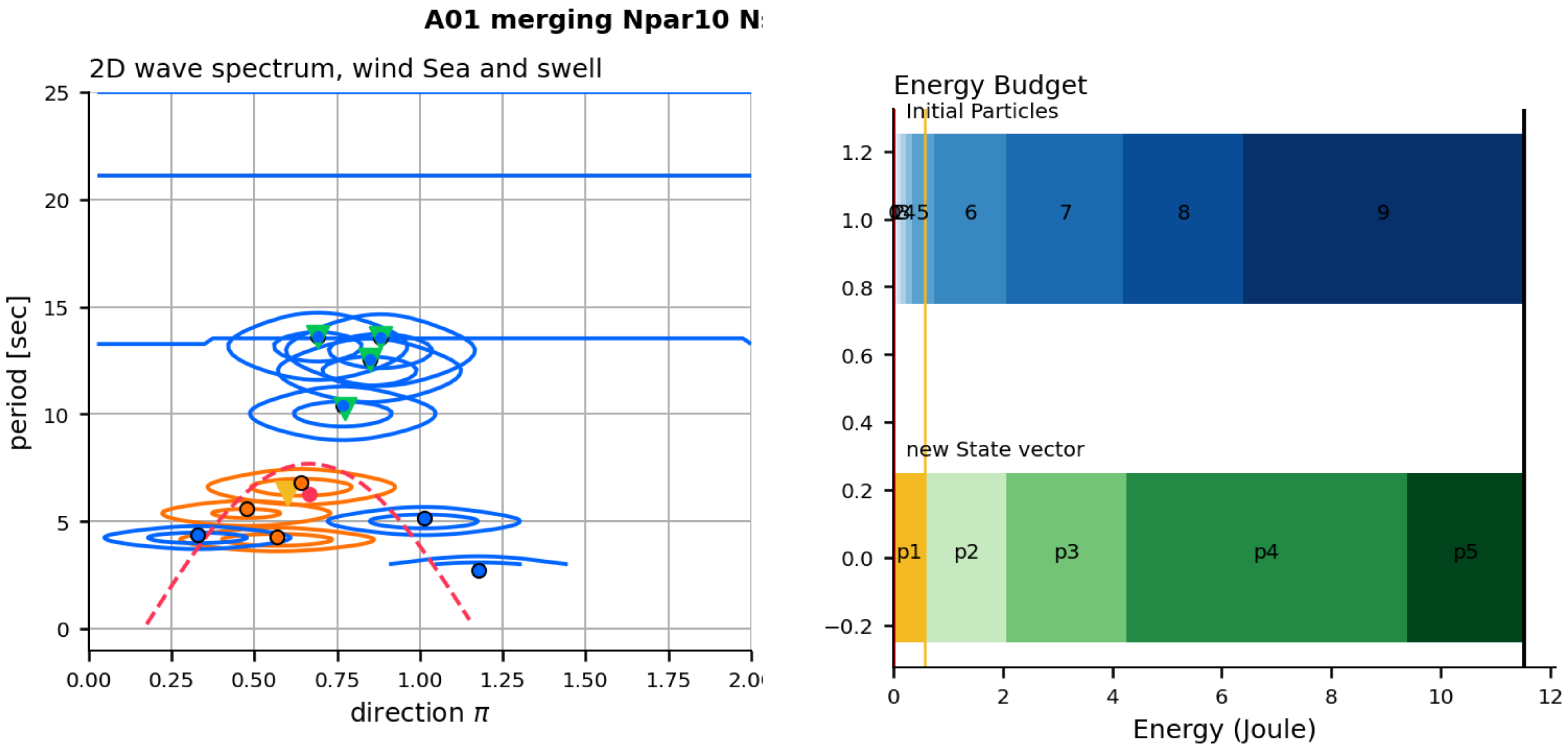
Growing waves under a moving fetch



Qualitatively reproduces results from Hell et al 2021:

- highest wave speeds and energy ahead of the high-test wind speeds.
- non-local effects under wave-growth conditions
- frequency and geometric dispersion not included yet.




A01 merging Npar10 N
2D wave spectrum, wind Sea and swell
period [sec]
direction π
Energy Budget
Initial Particles
new State vector
Energy (Joule)
p1
p2
p3
p4
p5