High-order Discontinuous Galerkin Methods and **Deep Reinforcement Learning with Application** to Multi-scale Ocean Modeling

Corbin Foucart PhD Defense, August 2, 2023



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Introduction

HDG Nonhydrostatic Ocean Modeling

Reinforcement Learning for Adaptive Mesh Refinement

Outline





Importance of nonhydrostatic dynamics:

"As horizontal resolutions increase, nonhydrostatic effects become increasingly strong and presently are detectable at the submesoscale [1-5] and in deep convection [6] ...

> ... few ocean circulation models presently have nonhydrostatic capability."

[Fox-kemper et al., Challenges and prospects in ocean circulation models, 2019]

[1] Mahadevan, 2006 [2] Hamlington et al., 2014 [3] Suzuki et al., 2016 [4] McWilliams, 1985 [5] Taylor and Thompson, 2023 [6] Marshall et al., 1997







Internal waves:



[1] Simmons et al., 2011





Subduction dynamics:

- Mechanisms of subduction are nonhydrostatic and not captured by regional models [2, 3] global models [1]
- Wind-driven surface stress can excite a dramatic dynamical response in the water column in terms of large-amplitude internal waves and strong vertical mixing [4, 5, 6]

Seiche-like free-surface dynamics



[1] Freilich & Mahadevan, JGR, 2021 [2] Pinardi et al, OM-2017 [3] Lermusiaux et al, OD-2013 [4] Calil, OD, 2017 [5] Kaempf, OD, 2017 [6] Kaempf, OD, 2019











Gale: March 27 00:00Z, W/SW

Nowcast : 19:00:00 27 Mar 2019

Wind Field

37N

36°30

Subduction dynamics:

- Mechanisms of subduction are nonhydrostatic and not captured by regional models [2, 3] global models [1]
- Wind-driven surface stress can excite a dramatic dynamical response in the water column in terms of large-amplitude internal waves and strong vertical mixing [4, 5, 6]
- Frontal subduction, mixed-layer instabilities in Belearic and Alboran seas [7]
- Dynamics important for ocean acoustics, nutrient transport, carbon subduction from the atmosphere at small horizontal length scales [1-7]







Why high-order methods?

Scalar advection equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{c}\phi) = \mathbf{0}$$

All three simulations: same computational cost [2]



High-order methods often provide more accurate solutions for the same computational cost [1, 2]

[1] Hesthaven, 2008 [2] Ueckermann, M.P., PhD Thesis





Effectiveness of high-order DG methods

DG methods: incredibly successful modeling a wide range of phenomena in computational physics [1, 2]

Importantly: effective in *under-resolved* regimes

- Stability and robustness for projection, fully-implicit schemes [3]
- Able to transport high-frequency features over long time-integration horizons without significant dissipation/dispersion [4]
- Efficient on modern computer architectures [5, 6]
- Well-suited to adaptive mesh refinement [2]

State-of-the-art, incompressible Navier-Stokes equations

[1] Hesthaven 2008 [2] Kronbichler and Persson, Springer, 2021a [3] Fehn et al., JCP, 2017 [4] Fehn et al., JCP, 2018a [5] Fehn et al., JCP, 2018b [6] Kronbichler and Wall, SIAM, 2018 [7] Nguyen et. al, JCP, 2009a







Apply high-order DG methods to nonhydrostatic modeling

Ocean models: few have nonhydrostatic capability, and **low-order**

- PSOM (Mahadevan, 2020)
- MERF v3.0 (Tang et al., 2021)
- SUNTANS, GVC (Fringer et. al 2006; Fringer et al., 2011; Yue et al., 2021)
- MIT GCM (Marshall et al., 1997)—
- CROCO-ROMS (Cambon et al., 2018)
- Oceananigans.jl (Ramadhan et al., 2021)

[1] Ueckermann, 2014, PhD Thesis; [2] Ueckermann & Lermusiaux, 2016; [3] Foucart et. al, 2018; [4] Pan et. al, 2019, [5] Pan et al., 2021, [6] Foucart et al., Ocean Modelling. in prep. 2023a.

State of the art, nonhydrostatic-capable models

Use of high-order DG methods for nonhydrostatic modeling: promising, but still in its infancy [1-6]



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[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.

Model domain & geometry



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Ocean Equations: temporal discretization [1, 2]

Ocean equations with a free-surface:

 $\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} &- \left(\nabla \cdot (\boldsymbol{\nu} \nabla \mathbf{u})\right) + \nabla p' + g \nabla_{xy} \eta \\ &= -\frac{1}{\rho_0} \int_z^{\eta} g \nabla_{xy} \rho' \, dz' - \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) + \frac{1}{\rho_0} \mathbf{f} \\ \frac{\partial \eta}{\partial t} &+ \nabla \cdot \left(\int_{-\mathcal{H}}^{\eta} \mathbf{u} \, dz\right) = 0 \\ &\nabla \cdot \mathbf{u} = 0 \\ \frac{\partial \rho'}{\partial t} &- \nabla \cdot (\kappa \nabla \rho') = -\nabla \cdot (\mathbf{u} \rho') + f_{\rho'} \end{aligned}$

where:

$$p = p_{hyd} + \rho_0 p', \qquad p_{hyd} = \int_z^{\eta} \rho g \, dz'.$$

 $\nu, \kappa \in \mathbb{R}^{d \times d}$ are diffusivity tensors

[1] Ueckermann, M.P., 2014 [2] **Foucart** et al., Ocean Modelling. in prep. 2023a.

$$\begin{aligned} & \mathbf{velocity\ predictor\ [3D]} \\ & \frac{\bar{\mathbf{u}}^{k+1}}{a\Delta t} - \left(\nabla \cdot \left(\nu \nabla \bar{\mathbf{u}}^{k+1}\right)\right) + \nabla p'^{,k} + g \nabla_{xy} \eta^{k} = \mathbf{F}_{\bar{\mathbf{u}}}^{k,k+1} \end{aligned} \\ & \mathbf{free-surface\ correction\ [2D]} \\ & \frac{\delta \eta^{k+1}}{a\Delta t} - \nabla \cdot \left(a\Delta tg\ (\eta^{k} + H)\ \nabla \delta \eta^{k+1}\right) = -\nabla \cdot \int_{-H}^{\eta^{k}} \bar{\mathbf{u}}^{k+1} \\ & \bar{\mathbf{u}}_{xy}^{k+1} = \bar{\mathbf{u}}_{xy}^{k+1} - (a\Delta t)g \nabla_{xy} \delta \eta^{k+1} \\ & \eta^{k+1} = \eta^{k} + \delta \eta^{k+1} \end{aligned} \\ & \mathbf{pressure\ correction\ [3D]} \\ & \nabla^{2} \delta p'^{,k+1} = \frac{\nabla \cdot \bar{\mathbf{u}}^{k+1}}{a\Delta t} \\ & \mathbf{u}^{k+1} = \bar{\mathbf{u}}^{k+1} - a\Delta t \nabla \delta p'^{,k+1}, \\ & p'^{,k+1} = p'^{,k} + \delta p'^{,k+1}. \end{aligned}$$

tracer evolution [3D]

$$\frac{{\rho'}^{k+1}}{a\Delta t} - \nabla \cdot \left(\kappa \nabla {\rho'}^{k+1}\right) - \nabla \cdot \left(\mathbf{u}^{k+1} {\rho'}^{k+1}\right) = \frac{{\rho'}^k}{a\Delta t} + f_{\rho'}.$$



Contribution: novel spatial discretization of ocean equations

- (nonhydrostatic and hydrostatic) [1, 2]
- - originally implemented in Python, then re-written in C++ for performance
 - multi-threaded implementation—parallelized HDG assembly/reconstruction
 - template meta-programming for dimension-specific compiler optimizations
 - suite of ~200 tests that verify implementations, optimal convergence rates for all solvers

[1] Foucart et al., 2021. [2] Foucart et al., Ocean Modelling. in prep. 2023a. [3,4] Nguyen et al., JCP. 2009a,b. [5] Fehn et al., JCP. 2017. [6] Fehn et al., JCP. 2018. [7] Kronbichler & Persson, Springer, 2021.

• Derived & implemented a new HDG spatial discretization of the free-surface ocean equations

• Incorporated ideas from classical HDG literature [3, 4] as well as modern results from DG literature pertaining to robust projection schemes for under-resolved incompressible flows [5, 6, 7]

• Implemented the discretization in a parallelized C++ framework tailored to HDG schemes





Spatial discretization: notation, finite element spaces

Mesh:

- Integer d: spatial dimension
- $\mathcal{T}_h = \bigcup_i K_i$: a finite collection of non-overlapping elements K_i discretizing $\Omega \subset \mathbb{R}^d$, with boundary Γ
- $\partial \mathcal{T}_h = \{\partial K : K \in \mathcal{T}_h\}$ interfaces and boundary edges of the elements, where ∂K is the boundary of element K
- Each edge $e \in \varepsilon^{\circ}$ or $e \in \varepsilon^{\partial}$, (interior and boundary edges)

Finite element spaces:

Let $\mathcal{P}^{p}(D)$ denote the set of polynomials of degree p on a domain D.

$$\begin{split} \mathbf{G}_{h}^{p} &= \left\{ \mathbf{G} \in \left[L^{2}(\Omega) \right]^{d \times d} : \mathbf{G} \Big|_{K} \in \left[\mathcal{P}^{p}(K) \right]^{d \times d} \forall K \in \mathbf{V}_{h}^{p} \\ \mathbf{V}_{h}^{p} &= \left\{ \mathbf{v} \in \left[L^{2}(\Omega) \right]^{d} : \mathbf{v} \Big|_{K} \in \left[\mathcal{P}^{p}(K) \right]^{d} \forall K \in \mathcal{T}_{h} \right\}, \\ W_{h}^{p} &= \left\{ w \in L^{2}(\Omega) : w \Big|_{K} \in \mathcal{P}^{p}(K) \forall K \in \mathcal{T}_{h} \right\}, \\ M_{h}^{p} &= \left\{ \mu \in L^{2}\left(\varepsilon_{h}\right) : \mu \Big|_{e} \in \mathcal{P}^{p}(e) \forall e \in \varepsilon_{h} \right\}, \end{split}$$

[1] Foucart et al., Ocean Modelling. in prep. 2023a.

 K_i



- $\in \mathcal{T}_h$







Weak formulation: velocity predictor

find: $(\bar{\mathbf{u}}_{h}^{k+1}, \bar{\mathbf{L}}_{h}, \hat{\mathbf{u}}_{h}) \in (\mathbf{G}_{h} \times \mathbf{V}_{h} \times \mathbf{M}_{h})$ such that

$$\begin{aligned} (\mathbf{G}, \, \bar{\mathbf{L}}_{h})_{\mathcal{T}_{h}} + (\nabla \cdot \mathbf{G}, \, \bar{\mathbf{u}}_{h}^{k+1})_{\mathcal{T}_{h}} - \langle \mathbf{G} \cdot \mathbf{n}, \, \hat{\mathbf{u}}_{h} \rangle_{\partial \mathcal{T}_{h}} &= 0 \\ \left(\mathbf{v}, \, \frac{\bar{\mathbf{u}}^{k+1}}{a\Delta t} \right)_{\mathcal{T}_{h}} - \left(\mathbf{v}, \, \nabla \cdot \left(\nu \bar{\mathbf{L}}_{h} \right) \right)_{\mathcal{T}_{h}} + \langle \mathbf{v}, \, \tau \left(\bar{\mathbf{u}}_{h}^{k+1} - \hat{\mathbf{u}}_{h} \right) \rangle_{\partial \mathcal{T}_{h}} \\ &= -a_{h} (\mathbf{u}^{k}, \mathbf{g}_{D}) - \mathrm{pg}_{h} \left(\mathbf{v}, \, p_{h}^{k} \right) - (\mathbf{v}, \, \mathbf{F}_{\rho'} + \mathbf{F}_{\eta} + \mathbf{F}_{\mathrm{cor}})_{\mathcal{T}_{h}} + (\mathbf{v}, \, \mathbf{F}_{t})_{\mathcal{T}_{h}} \\ &\langle \boldsymbol{\mu}, \, (-\nu \bar{\mathbf{L}}_{h}) \mathbf{n} + \tau (\bar{\mathbf{u}}_{h}^{k+1} - \hat{\mathbf{u}}_{h}) \rangle_{\partial \mathcal{T}_{h} \setminus \Gamma_{D}} + \left\langle \boldsymbol{\mu}, \, \widehat{b}_{h} \right\rangle_{\Gamma_{N}} = 0 \end{aligned}$$

for all $(\mathbf{G}, \mathbf{v}, \boldsymbol{\mu}) \in (\mathbf{G}_h \times \mathbf{V}_h \times \mathbf{M}_h)$.

Body forcing terms: $\mathbf{F}_{\rho'} = 1/\rho_0 \int_z^{\eta^k} g \nabla_{xy} \rho'^{,k} dz', \mathbf{F}_{\gamma}$

Advection term:

$$a_h(\mathbf{v},\mathbf{u}_h^k,\mathbf{g}_D) = -\left(
abla\mathbf{v},\,\mathbf{F}_a(\mathbf{u}_h^k)
ight)_{\mathcal{K}} + \left\langle \mathbf{v},\,\mathbf{F}_a^*(\mathbf{u}_h^k)
ight)_{\mathcal{K}}$$

Nonhydrostatic pressure gradient term:

$$\mathsf{pg}_h(\mathbf{v}, \pmb{p}_h^k) = -\left(
abla \cdot \mathbf{v}, \; \pmb{p}_h'^{,k}
ight)_{\mathcal{K}} + \langle \mathbf{v}, \; (\pmb{p}_h')^* \mathbf{n}
angle_{\hat{c}}$$

[1] **Foucart** et al., 2021 [2] **Foucart** et al., Ocean Modelling. in prep. 2023a.

$$\mathbf{F}_{\eta} = \mathbf{g} \nabla_{xy} \eta^{k}, \qquad \mathbf{F}_{cor} = f_{c} \hat{z} \times \mathbf{u}^{k}, \qquad \mathbf{F}_{t} = \frac{1}{a \Delta t} \mathbf{u}^{k},$$

Numerical flux definitions:

- $\left(\mathbf{u}_{h}^{k},\mathbf{g}_{D}
 ight)
 ight
 angle_{\partial K}$, $\mathbf{F}_{a}^{*}(\mathbf{u}_{h})=\mathbf{F}_{a}(\mathbf{u}_{h}^{k})_{\mathrm{upwind}}$
- $_{\partial \kappa}$, $(p_h')^* = \{\{p_h'\}\}$



Weak formulation: free-surface correction (dim - 1)

Define the gradient $\mathbf{q}_{\delta\eta} \equiv \nabla \delta \eta$. $\bar{\mathbf{U}}_h \equiv \int_{-H}^{\eta^k} \bar{\mathbf{u}}_{xv,h}^{k+1} dz$ find: $(\delta \eta_h^{k+1}, \mathbf{q}_{h,\delta\eta}, \hat{\delta \eta}_h) \in (W_h \times \mathbf{V}_h \times M_h)$ such that

$$\begin{pmatrix} \mathbf{v}, \frac{\mathbf{q}_{h,\delta\eta}}{a\Delta tg [\eta^k + H]} \end{pmatrix}_{\mathcal{T}_h} + (\nabla \cdot \mathbf{v}, \delta\eta_h^{k+1})_{\mathcal{T}_h} - \langle \mathbf{v} \cdot \mathbf{n}, \hat{\delta\eta}_h \rangle_{\partial \mathcal{T}_h} = 0, \\ \begin{pmatrix} w, \frac{\delta\eta_h^{k+1}}{a\Delta t} \end{pmatrix}_{\mathcal{T}_h} - (w, \nabla \cdot \mathbf{q}_{h,\delta\eta})_{\mathcal{T}_h} + \langle w, \tau \left(\delta\eta_h^{k+1} - \hat{\delta\eta}_h\right) \rangle_{\partial \mathcal{T}_h} = -d_h(w, \bar{\mathbf{U}}_h), \\ \langle \mu, \mathbf{q}_{h,\delta\eta} \cdot \mathbf{n} + \tau \left(\delta\eta_h^{k+1} - \hat{\delta\eta}_h\right) \rangle_{\partial \mathcal{T}_h} = \langle \mu, g_N \rangle_{\partial \mathcal{T}_h} \end{cases}$$

for all $(w, v, \mu) \in (W_h \times V_h \times M_h)$

Discrete depth-integrated divergence

$$d_h(w, \bar{\mathbf{U}}) = (w, \nabla \cdot \bar{\mathbf{U}})_{\kappa} = - (\nabla w, \bar{\mathbf{U}})_{\kappa} + \langle w, v \rangle_{\kappa}$$

[1] **Foucart** et al., 2021 [2] **Foucart** et al., Ocean Modelling. in prep. 2023a.

Numerical flux definition:

$$\left(\bar{\boldsymbol{\mathsf{U}}}\right)^* = \{\{\bar{\boldsymbol{\mathsf{U}}}\}\}$$

$$\left(\bar{\mathbf{U}}\right)^*\cdot\mathbf{n}_{\partial\kappa}$$



Weak formulation: pressure correction

Define the gradient of the pressure corrector q

find: $(\mathbf{q}_{\delta p'}, \delta p', \delta \hat{p}') \in (\mathbf{V}_h \times W_h \times M_h)$ such that

$$\begin{pmatrix} \mathbf{v}, \, \mathbf{q}_{\delta p'}^{k+1} \end{pmatrix}_{\mathcal{T}_{h}} + \left(\nabla \cdot \mathbf{v}, \, \delta p'^{,k+1} \right)_{\mathcal{T}_{h}} - \left\langle \mathbf{v} \cdot \mathbf{v} \right\rangle_{\mathcal{T}_{h}} \\ - \left(w, \nabla \cdot \mathbf{q}_{\delta p'}^{k+1} \right)_{\mathcal{T}_{h}} + \left\langle w, \, \tau_{p} \, \delta p'^{,k+1} \right\rangle_{\partial \mathcal{T}_{h}} - \left\langle w, \right\rangle_{\mathcal{T}_{h}} \\ \left\langle \mu, \, \mathbf{q}_{\delta p'}^{k+1} \cdot \mathbf{n} + \tau_{p} \, \left(\delta p'^{,k+1} - \delta \hat{p}' \right) \right\rangle_{\mathcal{T}_{h}} \end{pmatrix}$$

for all $(w, v, \mu) \in (W_h \times \mathbf{V}_h \times M_h)$

[1] **Foucart** et al., 2021 [2] **Foucart** et al., Ocean Modelling. in prep. 2023a.

$$\mathbf{q}_{\delta p'} = \nabla \delta p'.$$

Numerical flux definition: $(\bar{f u}^{k+1})^* = \{\{\bar{f u}^{k+1}\}\}$ $\cdot \mathbf{n}, \left. \widehat{\delta p'} \right\rangle_{\partial \mathcal{T}_h} = \mathbf{0},$ $\tau_{p}\widehat{\delta p'}\Big\rangle_{\partial \mathcal{T}_{h}} = \frac{1}{a\Delta t} \left[-\left(\nabla w, \, \bar{\mathbf{u}}^{k+1}\right)_{\mathcal{T}_{h}} + \left\langle w, \, \left(\bar{\mathbf{u}}^{k+1}\right)^{*} \cdot \mathbf{n} \right\rangle_{\partial \mathcal{T}_{h}} \right],$ $\delta \mathcal{T}_h ackslash \Gamma_d = 0$





Verification: convergence

 Spatial convergence test: method of manufactured solutions, inspired by [2].
 For each weak form (in 2D, 3D):

choose $\Upsilon = (\mathbf{u}, p', \eta, \rho')$

deduce the forcing term **f**

measure L^2 -error as (regular) mesh is refined

 Optimal p+1 convergence observed in both primal and gradient unknowns (HDG) (shown for the momentum equation, right)

[1] Foucart et al., Ocean Modelling. in prep. 2023a. [2] Hesthaven, Warburton, 2008



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Modeling Domain, Boundary Conditions



	top	bottom	sides
ū	Γ _N	Γ _N	Γ _D
\bar{W}	Γ_N	Γ_D	Γ _N
$\delta\eta$	_	_	Γ _N
$\delta p'$	Γ_D	Γ _N	Γ _N
ho'	Γ_N	Γ _N	Γ _N

[1] S. Vitousek and O.B. Fringer (2014), OM [2] Foucart et al., IEEE Oceans 2021 [3] Foucart et al., Ocean Modelling. in prep. 2023a.

Verification of NHS model: free-surface seiche

Initial Condition:

$$\eta(t=0)=a\cos(kx)$$

$$k = \frac{\pi}{L}$$





Verification of NHS model: free-surface seiche

Initial Condition, Parameters:



Analytical Solution: (linear gravity-wave theory)

$$u = ag \frac{k}{\omega} \frac{\cosh k(z+H)}{\cosh(kH)} \sin(kx) \sin(\omega t)$$
$$v = -ag \frac{k}{\omega} \frac{\sinh k(z+H)}{\cosh(kH)} \cos(kx) \sin(\omega t)$$

[1] S. Vitousek and O.B. Fringer (2014), OM [2] Foucart et al., IEEE Oceans 2021 [3] Foucart et al., Ocean Modelling. in prep. 2023a.

Solutions at one seiche period (t=T)

Numerical

Exact





3.1e-04

1.5e-04

0.0e+00



Initial condition, parameters:

$$\eta(t=0) = a \cos(kx)$$

 $H = 10$ m $L = 7.5$ m $a = 0.1$ m $T = 10^{-2}$ s



[1] S. Vitousek and O.B. Fringer (2014), OM [2] Foucart et al., IEEE Oceans 2021 [3] Foucart et al., Ocean Modelling. in prep. 2023a.

Verification of NHS model: free-surface seiche





Verification of NHS model: free-surface seiche

Depth profiles: agreement with NHS theory, deviation from HS prediction

Free-surface: numerical wave speed c



[1] Foucart et al., IEEE Oceans 2021 [2] Foucart et al., Ocean Modelling. in prep. 2023a.





Continuously-stratified internal seiche

Initial Condition:

Zero-free surface, stratified density perturbation



[1] S. Vitousek and O.B. Fringer (2014), OM [2] Foucart et al., IEEE Oceans 2021 [3] Foucart et al., Ocean Modelling. in prep. 2023a.

ation
$$\rho' = \frac{\Delta \rho}{2} \left[1 - \tanh\left(\frac{2 \tanh^{-1} \alpha_s}{\delta_{\rho}} (z + H/2 - \xi)\right) \right]$$





Continuously-stratified internal seiche

Interface wave speeds agree with theoretical values

$$c = \sqrt{\frac{g'}{2k}} \tanh\left(\frac{kH}{2}\right) f_i(k\delta\rho)$$

...over many different simulations with differing domain aspect ratios.

[1] S. Vitousek and O.B. Fringer (2014), OM [2] Foucart et al., IEEE Oceans 2021 [3] Foucart et al., Ocean Modelling. in prep. 2023a.





Additional verification / validation of HDG NHS model

Idealized mixed-layer Rayleigh Taylor Instability formation (shown last time)

- inflow velocity u = 50 cm/s pulls heavier water over lighter water
- Formation of RTI instabilities
- Mixing and re-stratification behind the front



[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.



Boundary Conditions

	top	bottom	inflow	ouflow
ū	Γ _N	Γ _N	Γ_D	Γ _N
\overline{W}	Γ_N	Γ_D	Γ_D	Γ _N
$\delta\eta$	_	_	Γ_N	Γ_N
$\delta p'$	Γ_D	Γ_N	Γ_N	Γ_N
ρ'	Γ _N	Γ _N	Γ _N	Γ _N

H = 50 m

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Idealized subduction: Rayleigh-Taylor instabilities

z [m]

Simulation: • Formation of RTI instabilities • Mixing and re-stratification behind the front

Modeling Domain

 $u(x = 0, t) = 50\hat{x} \text{ cm/s}$ ho' = 0.1z [m] $ho'(\mathbf{x},t=0)=0$ H = 50 mho'=0 $x_{L} = 0$ $x_R = 30 \text{ km}$

[MSEAS group, CALYPSO Sea Experiment 2022]



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Additional verification / validation of HDG NHS model

0 .

-10 -

-20 -

-30 -

-40 ·

-50 -

0

0

-10

-20

-30

-40

-50

Vertical Velocity -20 -30 -40

-50

0

Density Perturbation

Horizonatal Velocity

HDG



- **Goal:** verify diffusive physics by comparison to a legacy finite volume (FV) code
 - 2D incompressible Navier-Stokes solver with Boussinesq approximation

parameters					
	HDG	FV	units		
N_x , N_z	(25, 10)	(540, 25)			
$ u_{X}$	$1\cdot 10^2$	$1\cdot 10^2$	m^2/s		
ν_z	$8 \cdot 10^{-3}$	$8 \cdot 10^{-3}$	m^2/s		
Δt	100	100	S		
order	4	2			

[1] Foucart et al., Ocean Modelling. in prep. 2023a.

t = 6 hrs 2.29 (FV)











Additional verification / validation of HDG NHS model



- **Goal**: verify diffusive physics by comparison to a legacy finite volume (FV) code
 - 2D incompressible Navier-Stokes solver with Boussinesq approximation
- Differences explainable by free surface
- Excellent agreement with FV code
- HDG: significant reduction of cost (high-order)
 - 540 x 25 grid (FV)
 - 25 x 10 elements (polynomial order 4)



[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.

t = 10 hrs

HDG







Internal Solitary Wave Generation

Strongly-stratified flow over "tall" seamount:



- 200km x 1000m domain
- ISWs propagate away from the seamount
- Nonlinear ISW train develops in leading left-propagating wave starting around 1.25 tidal cycles
- Qualitative agreement with expected nonhydrostatic behavior

Low order simulations **did not** capture ISW train

[1] S. Vitousek and O.B. Fringer 2014 [2] Buijsman, et al. 2010 [3] Foucart et al., 2018

Normalized density perturbation ρ'/ρ_0 (Top 20% of domain)

Initial value



After 0.5 tidal cycles



After 1 tidal cycle



After 1.5 tidal cycles







Internal Solitary Wave Generation



[1] Foucart et al., 2018



Application: 2D model nesting within a large hydrostatic code (MSEAS-PE)

Region of investigation:

- Salmon-colored line: denotes a vertical section in the Alboran Sea along which wind-driven instabilities were observed in the hydrostatic MSEAS PE simulations
- The section starts in the west along the northern edge of the West Alboran Gyre and extends to the east-bynortheast out of the gyre towards the Spanish coast.
- Implemented 2D HDG NHS model nesting and initialization from real data
- Goal: model instabilities in the mixed layer and compare to HS simulation output

Modeling domains



Modeling domain for model nested runs in the Alboran Sea showing the MSEAS-PE domain (shaded, black), and the HDG NHS nested modeling domain (blue) in 2D (center slice) and 3D (box).





2D model nesting in the Alboran sea

Model comparison after wind event

- HDG NHS initialized on March 25, run for 5 days
- Same parameters and effective resolution as hydrostatic MEAS-PE model (500 m)
- Gale: March 27 2019

Modeling Domain

March 27, 2019



[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.



NHS model: boundary conditions

	top	bottom	sides
ū	Γ _D	Γ _D	Γ _D
\bar{w}	Γ _N	Γ_D	Γ _D
$\delta\eta$	-	-	Γ_N
$\delta {m p}'$	Γ _D	Γ _N	Γ _N
ρ'	Γ _D	Γ_D	Γ _D





- hydrostatic MEAS-PE model
- domain
- hydrostatic model once again



simulation time: 89.8 hours





HDG (nonhydrostatic)

2D model nesting in the Alboran sea



$$\frac{\partial \rho'}{\partial z}$$
 - measure of instability red - unstable, blue - stable

Initialization from Alboran sea data (MSEAS-PE)

simulation time: 89.2 hours



[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.



3D Model Nesting in the Alboran Sea

Region of investigation:

- Modeling domain: denotes a section in the Alboran Sea along which **wind-driven instabilities** were observed in the hydrostatic MSEAS PE simulations
- The section starts in the west along the northern edge of the West Alboran Gyre and extends to the east-by-northeast out of the gyre towards the Spanish coast.
- Implemented 3D HDG NHS model nesting and initialization from real data
- Goal: model instabilities in the mixed layer and compare to HS simulation output as well

[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.

modeling domains



Modeling domain for model nested runs in the Alboran Sea showing the


Density perturbation, domain to scale



[1] Foucart et al., Ocean Modelling. in prep. 2023a.







Domain scaled by factor of 300 in z



[1] Foucart et al., Ocean Modelling. in prep. 2023a.



• In 3D, interpretation can be very sensitive to the visualization







[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.







[1] Foucart et al., Ocean Modelling. in prep. 2023a.





[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.

Density perturbation between 2.4, 2.5 kg/m³







Overhang instability



What are the vertical velocities?

[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.









Ideally, we would like to visualize both together



[1] **Foucart** et al., Ocean Modelling. in prep. 2023a.





What does this model let us do?

- Perform zonal investigations of nonhydrostatic behavior
 - Areas with steep bathymetry [1], [5], [6]
 - Regions experiencing wind stress [1], [3], [4]
- Validate hydrostatic models
 - Determine when hydrostatic models are capable of resolving the correct length/time scales of ocean processes, and when they aren't [1], [5], [7-9]
- Discover parametrization for incorporation into large legacy hydrostatic models / climate models
 - Statistical descriptions of the same (Oceananigans.jl) [7]
- Hydrostatic/nonhydrostatic domain splitting
 - Work already started in our group [9]
 - DG/HDG boundary conditions advantageous for such approaches

[1] Foucart et al., Ocean Modelling. in prep. 2023a. [2] Freilich & Mahadevan, JGR, 2021 [3] Calil, OD, 2017 [4] Kaempf, OD, 2019 [5] Vitousek and Fringer 2014 [6] Buijsman, Kanarska, and McWilliams 2010 [7] Ramadhan, et. al (2022) [8] Foucart et al., 2018 [9] A. Karthik, MSEAS, SM Thesis



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	5448 (45.4) (54.5) (44.5) (44.5) (44.5) (44.5) (44.5) (44.5)
ang	
MED	380



Introduction

HDG Nonhydrostatic Ocean Modeling

Reinforcement Learning for Adaptive Mesh Refinement

Outline





Deep reinforcement learning for adaptive mesh refinement

Motivation:

- machine learning excels at learning latent patterns from large datasets in the absence of a model [1]
- a PDE is often an excellent model, and numerical methods provide stability, consistency, and convergence guarantees
- using machine learning to directly learn solutions to PDEs is subject to demonstrable failure modes, and often generalizes poorly [2]

Idea:

- use machine learning to improve heuristic elements of numerical solvers for which we don't have a good model
- adaptive mesh refinement is one such aspect

[1] Bishop, 2006 [2] Krishnapriyan et al., 2021 [3] Foucart et al., JCP. 2022.



Adaptive mesh refinement (AMR)

Pseudocolor Var: solution – 20.32

- 14.91

-9.514

- 4.113

1.288

Max: 20.32 Min: -1.288

Mesh Var: mesh

PDE:

$$\nabla \cdot (\mathbf{c}u) = f$$

$$u = g_D \qquad \text{on } \Gamma_{\text{inflow}}$$

Idea: refine mesh only "where something is happening"

AMR strategies: SOLVE ESTIMATE MARK REFINE (difficult, heuristic) [1]

[1] T. Plewa et al., 2005; De Sterck et al., 2008



Mesh, Numerical solution



Adaptive mesh refinement strategies are difficult and heuristic

Idea: Use deep reinforcement learning to find a good strategy













Reinforcement learning

Agent: interacts with environment at discrete time intervals

- takes action a_t on state s_t
- receives reward r_{t+1}
- state transitions to s_{t+1}

Markov decision process: tuple (S, A, T, R, γ) S - set of possible states, "state space" A - set of possible actions, "action space" $T(s', a, s) = \operatorname{prob}(s_{t+1} = s' | s = s_t, a = a_t)$ R - set of possible rewards $\gamma \in [0, 1]$ - time discount factor

[1] Sutton and Barto, 2018; D. Silver, 2015



Goal:

choose stochastic policy $\pi \colon S \to A$ that maximizes expected reward

$$Q_t(s, a) = \mathbb{E}_{\pi} \left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \mid S_t = s, A_t
ight]$$

over an infinite time horizon





Deep reinforcement learning

"Deep" RL:

- represent value function as neural network
- use each reward signal (experience) to update network during training
- once trained, agent is "deployed" by querying policy network for recommendation based on current state and action
- neural networks are universal function approximators [3] and can learn arbitrarily complex policies

[1] Sutton and Barto, 2018 [2] D. Silver, 2015 [3] Kornik et al., 1989



goal:

choose stochastic policy $\pi: S \to A$ that maximizes expected reward

$$Q_t(s, a) = \mathbb{E}_{\pi} \left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \mid S_t = s, A_t
ight]$$

over an infinite time horizon





How can we make our numerical solver "play against itself?"

Original problem:

$$abla \cdot (\mathbf{c}u) = f$$

 $u = g_D$ on Γ_{inflow}

Weak formulation [1]:

find u_h such that

$$-\left(
abla w, \mathbf{c} u_h
ight)_{\Omega} + \langle w, \, \hat{u}_h(\mathbf{c}\cdot\mathbf{n})
ight
angle_{\partial\Omega} = (w, f)_{\Omega}$$

for all $w \in \mathcal{P}^p$, the space of discontinuous polynomials of order p on each element





Increasing conformity upon refinement

Key idea:

- underlying solution to PDE is **continuous**



[1] Foucart et al., JCP. 2022.



Increasing conformity upon refinement

Key idea:

- underlying solution to PDE is **continuous**



[1] Foucart et al., JCP. 2022.



Designing the reward function

"Change in *U_h* as a result of refinement"



[1] Foucart et al., JCP. 2022.

"Computational cost incurred"





Single RL agent



[1] Foucart et al., JCP. 2022.

Training







- the local solution
- the interface jumps over the cell boundary
- the average interface jump over all mesh interfaces
- the current usage of computational resources
- any PDE-specific features the user wishes to provide

Training



Action space:



do nothing

coarsen



- the local solution
- the interface jumps over the cell boundary
- the average interface jump over all mesh interfaces
- the current usage of computational resources
- whatever PDE-specific features you want to provide

Training







- the local solution
- the interface jumps over the cell boundary
- the average interface jump over all mesh interfaces
- the current usage of computational resources
- whatever PDE-specific features you want to provide

Training



refine cycle 1: 4/25 cells used





- the local solution
- the interface jumps over the cell boundary
- the average interface jump over all mesh interfaces
- the current usage of computational resources
- whatever PDE-specific features you want to provide

Training







- the local solution
- the interface jumps over the cell boundary
- the average interface jump over all mesh interfaces
- the current usage of computational resources
- whatever PDE-specific features you want to provide

Training







Training

This is the numerical solver "playing against itself" Over time, it learns a good refinement strategy.



5000 10000 15000 20000 25 Training timestep



Walk every cell with the RL-agent



[1] Foucart et al., JCP. 2022.

Deployment:

and refine according to its recommendation.



Steady-state advection equation

$$\nabla \cdot (\mathbf{c}u) = f$$

$$u = g_D \quad \text{on } \Gamma_{\text{inflow}}$$

$$\text{velocity } \mathbf{c} = 1$$

$$\Gamma_{\text{inflow}} = \{x \in \Gamma : \mathbf{c} \cdot \mathbf{n} \le 0\}$$

*at no point during training or deployment do we make use of the exact solution

[1] Foucart et al., JCP. 2022.

Proof of concept: smooth jump test case

Exact solution*







Trained model deployment

RL Agent, 25 cell budget



Deep RL for AMR



Test against a typical AMR implementation (gradient-based, 50/50 bulk-refinement)



[1] Foucart et al., JCP. 2022.



Degrees of freedom



Does it generalize?

 $-1.5 \cdot$

Same trained RL model as in previous example



- No additional training
- Apply it to same PDE, but with new boundary conditions and forcing function
- Does it still recommend a good mesh?



[1] Foucart et al., JCP. 2022.



-2

-1

-3







Time-dependent problems

Sommerfeld wave equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$

initial condition:

$$u_0 = \exp\left(\frac{1}{2\sigma^2}(x-\mu)^2\right)$$
$$\sigma^2 = 0.25 \qquad \mu = -4$$

RL agent strategy preserves solution features, at a fraction of the cost.

[1] Foucart et al., JCP. 2022.





Higher-dimensional problems

steady-state advection equation:

$$abla \cdot (\mathbf{c}u) = 0 \quad \text{in } \Omega = (0, 1)^2,$$
 $u = g_D \quad \text{on } \Gamma_{\text{inflow}}$

circular, counter-clockwise velocity field cylindrical gen. of the "smooth jump"

$$\mathbf{c} = \frac{1}{\|x\|_2} (-x_2, x_1)$$

$$g_D = \begin{cases} 1 - \tanh[\alpha(1 - 4(x - x_0))], & x_1 \in [0, 1], x_2 = 0\\ 0, & \text{otherwise} \end{cases}$$

[1] Foucart et al., JCP. 2022.





RL agent suggests more conservative refinement

AMR heuristic (gradient-based)



[1] Foucart et al., JCP. 2022.









0.5

The RL agent's strategy





[1] Foucart et al., JCP. 2022.



70

How does the RL policy compare to the AMR heuristic?



[1] Foucart et al., JCP. 2022.

RL agent learned to refine where the steep gradient meets the outflow boundary

L²-Error

We never "told" it how to do this

In fact, recall that the agent never knows where it "is"





Advances: more complicated PDE, numerical scheme, solution features

Advection diffusion, mixed boundary conditions

$$\nabla \cdot (\mathbf{c}u) - \nabla \cdot (\kappa \nabla u) = f, \qquad \text{in } \Omega$$

$$u = g_D$$
, on Γ_D



[1] Nguyen et al., JCP 2009a. [2] Foucart et al., JCP. 2022.

Discretized with a fourth-order hybridizable


More complicated, time-dependent dynamics

2D ring advection [1] **test case**:



[1] Kulkarni & Lermusiaux. JCP. 2019

Figure 19: Unsteady reversible 2D ring advection. Numerical solution on a 64×64 uniform grid.



-0.1

More complicated time-dependent dynamics

Train on a much simpler example: advection of Gaussian pulse



(a) Initial condition u_0

[1] Foucart et al., JCP. 2022.

(b) Convective velocity *c*



More complicated time-dependent dynamics: 2D ring advection

- The RL agent is able to accurately preserve the shape of the ring over time integration
- Practically same accuracy as the AMR heuristic (Kelly bulk refinement), but does so at a fraction of the cost of the heuristic in terms of number of cells







Refine Uniform \mathbf{AMR} DRL A

Table 3: Unsteady reversible 2D ring advection. Comparison of numerical errors at final time T = 1. The evolution in time of the number of active cells is provided in Figure 21.

[1] Foucart et al., JCP. 2022.

ement method	L^2 -error	Percent change
mally refined mesh (4096 cells), ground truth	$1.8316 \cdot 10^{-2}$	-
Heuristic (Kelly)	$1.9553 \cdot 10^{-2}$	6.8%
Agent	$1.9630 \cdot 10^{-2}$	7.2%



Effective AMR policies can be discovered directly from numerical simulation using deep reinforcement learning. More complicated time-dependent dynamics

- the RL policy network is trained directly through experience by numerical simulation on small problems, and can be deployed on much larger problems
- learns a local relationship, and therefore robust to overfitting on any particular feature seen during training
- the deep-RL AMR technique is not specific to any dimension, PDE, or numerical solver
- at no point during training or model deployment do we ever use an exact solution or "ground truth"

Deep RL for AMR: summary

Train on a much simpler example: advection of Gaussian pulse More complicated time-dependent dynamics: 2D ring advection The RL agent is able to accurately preser the shape of the ring over time integrat Practically same accuracy as the AMB houristic (Kelly bulk refinement), but does so at a fraction of the cost of the heuristic in (a) Initial condition no (b) Convective velocity c 304 400 400 800 1 Current numerical solution: Observation space Action space: How does the RL policy compare to the AMR heuristic AMR heuristi Advances: more complicated PDE, numerical scheme, solution features RL agent learned to refine the steep gradient meet outflow boundary vection diffusion, mixed boundary conditions We never "told" it how " on F_N, In fact, recall that the ager on Γ_D , knows where it "is"







Publications

Scientific machine learning:

Foucart, C., A. Charous, and P.F.J. Lermusiaux, 2022. Deep Reinforcement Learning for Adaptive Mesh Refinement. Journal of Computational Physics,. arXiv preprint

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DG-FEM, ocean modeling:

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and P.F.J. eling for , 22-25



Nonhydrostatic HDG Ocean Modeling [2], [3]

- Development and implementation of a novel HDG spatial discretization of the hydrostatic & nonhydrostatic ocean equations with a free surface
- Wrote a parallelized C++ library implementation
- Verification of NHS / HS model with results from linear wave theory
- Idealized simulations of nonhydrostatic behavior (subduction, internal solitary waves)
- Implemented model nesting in the MSEAS-PE code for use with real ocean data in 2D and 3D
- Conducted preliminary investigations of nonhydrostatic behavior in the Alboran Sea

Miscellaneous DG/HDG contributions:

- Quadrature-free HDG operator formulation & matrix-free schemes [5]
- Computational considerations for treatment of the singular Poisson equation
- UQ: EnKF for HDG ensembles, Bayesian inversion of PDE coefficients using MCMC with DG schemes
- Parallel and multi-threaded computing approaches for HDG schemes [4], [5]

[1] Foucart et al., JCP, 2022. [2] Foucart et al., Ocean Modelling. in prep. 2023a. [3] Foucart et al., IEEE Oceans 2021. [4] Foucart et al. IEEE Oceans, 2018. [5] Foucart, SM Thesis, 2019.

Summary of contributions

Deep Reinforcement Learning for AMR [1]

- Formulated adaptive mesh refinement as a reinforcement learning problem
- Conceived and implemented neural network architectures to learn to solve the reinforcement learning problem, without training data or an exact solution
- Wrote a binding language between custom AMRcapable DG/HDG solvers and machine learning libraries
- Showed the resultant trained policies to be competitive or better than many common AMR heuristics, over a wide range of PDEs and test cases





Acknowledgements

- Prof. Nicholas Patrikalakis, Prof. Jaime Peraire
- under grants OCE-1061160 (ShelfIT) and EAR-1520825 (NSF-ALPHA)

• Committee Members: Prof. Pierre F.J. Lermusiaux, Dr. Cuong Nguyen, Prof. Anthony Patera,

• **Funding:** Office of Naval Research for support throughout this research and Ph.D. under grants N00014-15-1-2626 (DRI-FLEAT), N00014-18-1-2781 (DRI-CALYPSO), and N00014-20-1-2023 (MURI ML- SCOPE), the Defense Advanced Research Projects Agency (DARPA) for support under grant N66001-16-C- 4003 (POSYDON), and the National Science Foundation for support

• Administrative staff: Lisa Maxwell, Leslie Regan, Una Sheehan, Saana McDaniel, Kate Nelson



Thank you, MSEAS









Thank you, MSEAS



Thank you, Abhinav

















Thank you!



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Extra slides



Free surface boundary conditions

8. Appendix A

Derivation of free-surface boundary conditions

The conceptual basis of the projection scheme is the idea that we can define a "total effective nonhydrostatic pressure" which has component due to the free-surface η and a component due to the nonhydrostatic pressure p'.

$$\mathbf{P}_{\rm eff}' = p' + g\eta,\tag{46}$$

which explains the terms $\nabla P' = \nabla p' + g \nabla \eta$ in the momentum equation (1). The free-surface corrector and intermediate projection step enforces the free-surface continuity equation and projects out the velocity divergence due to the free-surface pressure $g\eta$. The pressure-corrector step projects out the velocity divergence due to the nonhydrostatic pressure p'.

To enforce the free-surface evolution equation (3), we

$$\frac{\eta^{k+1}}{a\Delta t} + \nabla \cdot \int_{-H}^{\eta} \left(\bar{\boldsymbol{u}}^{k+1} - a\Delta t \nabla_{xy} \left(g\delta\eta^{k+1} \right) \right) dz = \frac{\eta^{k}}{a\Delta t}
\Rightarrow \frac{\delta\eta^{k+1}}{a\Delta t} - \nabla \cdot \left(a\Delta tg \left[\eta^{k} + H \right] \nabla \delta\eta^{k+1} \right) = -\nabla \cdot \int_{-H}^{\eta} \bar{\boldsymbol{u}}^{k+1} dz.$$
(47)

For a Dirichlet boundary condition on the velocity u^{k+1} , making use of the definition of $\overline{\bar{u}}^{k+1}$, we have

$$\nabla \delta \eta^{k+1} = \frac{\bar{\boldsymbol{u}}^{k+1} - \bar{\bar{\boldsymbol{u}}}^{k+1}}{a\Delta tg}$$
$$\Rightarrow g_{N,\delta\eta} = \nabla \delta \eta^{k+1} \cdot \boldsymbol{n} =$$

which enforces that the horizontal component of the second intermediate velocity $\bar{\bar{u}}^{k+1}$ has the value $g_{D,u}$ on the boundary Γ_D after the intermediate updates⁴. In the case where we were able to enforce that $\bar{u}^{k+1} = g_{D,u}$ exactly, this reduces to a zero-Neumann condition; however, since HDG methods may only impose boundary conditions weakly through the edge-space M_h^p , the value $g_{N,\delta\eta}$ may not be exactly zero numerically⁵.

approximate
$$\boldsymbol{u}^{k+1}$$
 by $\bar{\boldsymbol{u}}^{k+1} = \bar{\boldsymbol{u}}^{k+1} - a\Delta t \nabla_{xy} \left(g\delta\eta^{k+1}\right)$:

$$\frac{1}{a\Delta tg} \left(\bar{\boldsymbol{u}}^{k+1} - \boldsymbol{g}_{D,\boldsymbol{u}} \right) \cdot \boldsymbol{n}$$
(48)



Pure Neumann problem: convergence

Singular system

- Arises in pressure-poisson equation
- Rank-one deficient
- Several approaches to treat singularity [2]:
 - point constraint
 - penalty method
 - subspace projection
- All converge optimally (but at different costs), no rigorous comparison has ever been done [1]



[1] Foucart et al., JCP. in prep. 2023b. [2]

P. Bochev and R. B. Lehoucq. SIAM Review, 2005







Pure Neumann problem: benchmarking

Singular system

- Several approaches to treat singularity:
 - point constraint
 - penalty method
 - subspace projection

Compare their performance in terms of iterative solver iterations





Pure Neumann problem: benchmarking

Singular system

- Several approaches to treat singularity:
 - point constraint
 - penalty method
 - subspace projection

Solver iterations can be misleading due to the cost of applying each iteration; measure error as a function of wall-clock time to solution.

Subspace projection is unambiguously the best, especially at high-order





Deep reinforcement learning: training and deployment

"deep" RL:

- represent value function as neural network
- use each reward signal (experience) to update network during **training**
- once trained, agent is "**deployed**" by querying policy network for recommendation based on current state and action
- neural networks are universal function approximators (Kornik et al., 1989) and can learn arbitrarily complex policies

(Foucart et al., JCP-2022-sub)







Application: 2D model nesting within a large hydrostatic code (MSEAS-PE)

Region of investigation:

- Black line: denotes a section in the Alboran Sea along which winddriven instabilities were observed in the hydrostatic MSEAS PE simulations
- The section starts in the west along the northern edge of the West Alboran Gyre and extends to the east-by-northeast out of the gyre towards the Spanish coast.
- Implemented 2D HDG NHS model nesting and initialization from real data
- Goal: model instabilities in the mixed layer and compare to HS simulation output

INHS model: boundary conditions				
	top	bottom	sides	
ū	Γ _D	Γ _D	Γ _D	
\bar{w}	Γ _N	Γ_D	Γ _D	
$\delta\eta$	-	-	Γ _N	
$\delta {m p}'$	Γ _D	Γ _N	Γ _N	
ρ'	Γ _D	Γ _D	Γ _D	

NUC model houndary conditions

[1] Foucart et al., Ocean Modelling. in prep. 2023a.



MSEAS-PE (hydrostatic)

