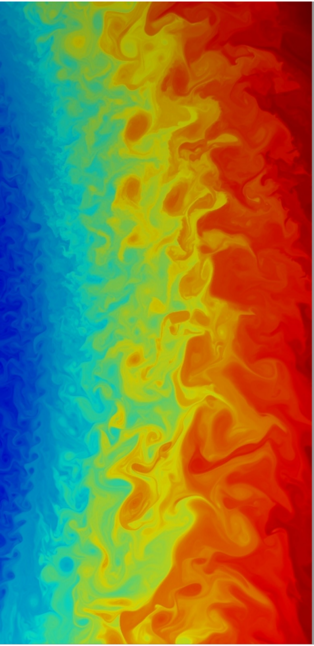

Can we improve the numerical formulation used in MPAS-Ocean?

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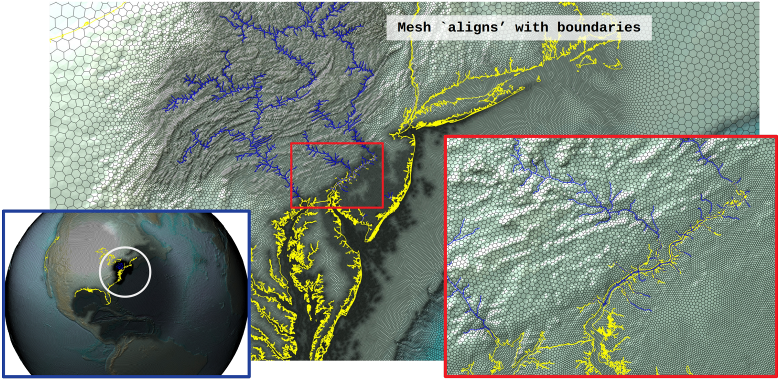
ESMD Meeting: October, 2020

‘Aggressive’ variable resolution configurations?

Expect that future MPAS-O configurations will employ **very ‘aggressive’ variable resolution meshes** $\rightarrow$ capture multi-scale ‘global-to-coastal’ dynamics.

- O(100km) global mesh $\rightarrow$ O($\leq$ 1km) embedded coastal meshes.



**Embedded mid-Atlantic coastal-zone: ICoM project, Engwirda et al, 2020.

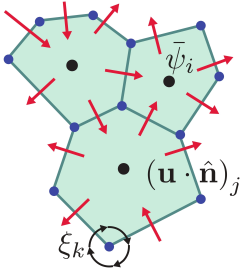
- How accurate is the ‘TRiSK’ formulation used in MPAS-O in such cases?
- Can this be improved on? (2nd/3rd-order accuracy, general meshes, etc)

How accurate is the TRiSK scheme?

The **TRiSK** scheme is a mimetic finite-difference/volume formulation based on unstructured (Voronoi) meshes:

- Conserved tracers stored within cells.
- Horizontal velocity DoF staggered at cell edges.
- Rotational DoF evaluated at polygon vertices.

TRiSK is a low(er)-order discretisation — it does not use polynomial reconstruction / interpolation operators, etc, but relies on staggered DoF placement.

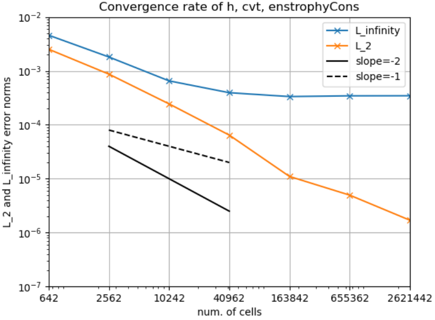


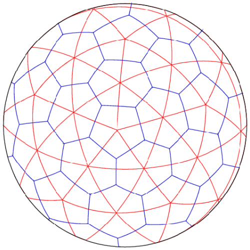
**A unified approach to energy conservation and potential vorticity dynamics for arbitrarily-structured C-grids, Ringler et al, 2010

To test behaviour / discrete order-of-accuracy, we have conducted a **grid convergence study** — benchmark cases run on progressively refined meshes, with documentation of error metrics.

How accurate is the TRiSK scheme?

Using a sequence of quasi-uniform icosahedral meshes (CVT optimised), the TRiSK-SWE (shallow-water) dycore has been used to assess convergence wrt. layer thickness:





**Quasi-uniform icosahedral mesh sequence — 'best-case' for spherical grids

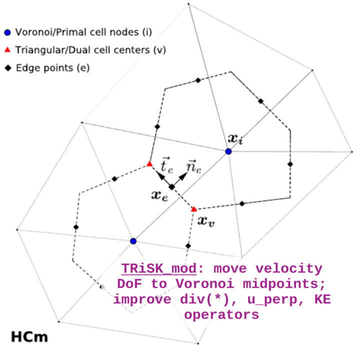
- In $\|\cdot\|_2$, fluid thickness shows approx. 2nd-order accurate behaviour.
- BUT, in $\|\cdot\|_{\text{inf}}$ (worst-case), convergence is less-than 1st-order — in fact, **convergence stalls completely at high-resolution!**

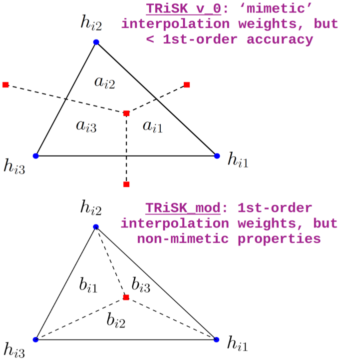
Opportunities to improve the performance of MPAS-O (espec. for variable-res. meshes, etc), by revisiting the TRiSK formulation.

**Convergence of a 'modified' TRiSK scheme, Calandrini et al, 2020.

A ‘modified’ TRiSK formulation

A ‘modified’ TRiSK formulation is currently being investigated (Calandrini, et al), adopting new velocity DoF placement + alternative weights / reconstructions to improve order-of-accuracy:





Modified scheme achieves $\geq$ 1st-order convergence in $\|\cdot\|_{\mathbf{inf}}$, but sacrifices some ‘mimetic’ aspects of TRiSK (loss of exact energy conservation, geostrophic balance, PV compatibility).

Currently working to understand accuracy vs loss-of-mimetic trade-offs — may provide near-term improvements for MPAS-O accuracy.

**Accuracy analysis of mimetic finite volume operators on geodesic grids and a consistent alternative, Peixoto, 2016.

A full ‘upgrade’ to TRiSK

Over the long(er)-term, achieving better than 1st/2nd-order accuracy in MPAS-O is desirable...

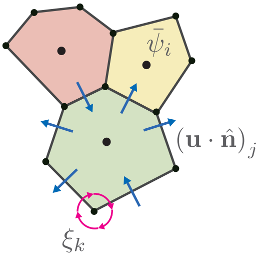
- Propose a new numerical-methods / computational-physics research effort to ‘upgrade’ the TRiSK formulation using new(er) discretisation formalism (Discontinuous Galerkin, Exterior Calculus, etc)
- Aim to upgrade ‘concept’ of the existing TRiSK scheme.
- Preserve desirable aspects of TRiSK: Voronoi-type meshes, staggered tracer, velocity, vorticity DoF, analysis workflows, etc.
- Upcoming Ocean-NGD effort intends a full rewrite of the overall MPAS-O framework.

A full 'upgrade' to TRiSK

Re-formulate TRiSK to achieve higher-order accuracy on general meshes.

Higher-order accuracy → better dynamics (waves, eddies, etc), coarser meshes, etc.

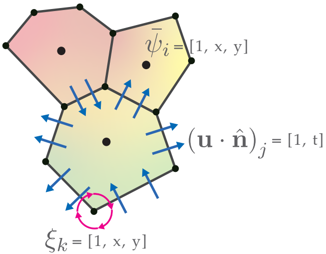
TRiSK v0:



Finite-difference / Finite-volume:

- **Low order accurate**: 2nd-order only if 'perfect' Cartesian mesh, 1st-order on sphere or if variable resolution.
- Piecewise **constant** approximations: edge fluxes, cell basis functions, etc.
- Nice 'mimetic' properties: geostrophic modes, enstrophy, energy, etc.

TRiSK-DG:



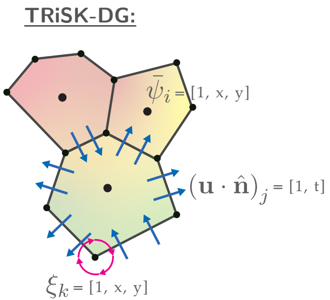
'Staggered' Discontinuous-Galerkin:

- **Higher-order accurate**: 2nd/3rd-order polynomial basis functions, general unstructured meshes.
- Piecewise **linear** (or better) approx.: edge fluxes, cell interpolation, etc.
- Same staggered variables as TRiSK → opportunity for same 'mimetic'-ness.

A full 'upgrade' to TRiSK

Higher-order accuracy $\rightarrow$ better dynamics (waves, eddies, etc), coarser meshes, etc.

- **Idea**: replace piecewise constant approx. of TRiSK-v0 with polynomial basis functions.
- More velocity DoF per edge, more SSH + tracer DoF per cell, **BUT** with same staggering as TRiSK-v0.
- Use 'reconstructed'-DG formulation $\rightarrow$ assemble high-order approx. to cell basis functions using 'compact' stencil of neighbouring cell polynomials.
- For example, quasi 3rd-order accuracy (quadratic basis) for $\mathrm{grad}(\cdot)$, $\mathrm{div}(\cdot)$, $\mathrm{curl}(\cdot)$, etc, assembled from linear DG expansions per cell.
- Discrete Exterior Calculus approach $\rightarrow$ details for another day!
- While dycore involves high-order DoF, output low-order DoF to file: preserve mesh, model I/O, visualisation, analysis from existing MPAS framework.

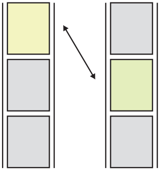


**Allow variation in velocity 'along' cell edges, as well as for SSH, T, S, etc 'within' cells: $\geq$ 2nd-order accuracy.

A full ‘upgrade’ to TRiSK

Higher-order basis functions $\rightarrow$ ‘dense’ computational kernels, matrix operations.

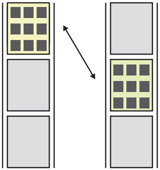
TRiSK v0:



Finite-difference / Finite-volume:

- Operate on each DoF individually via **for** loops, etc.
- Slower scattered memory accesses, cache misses, etc.
- No BLAS/CUDA-style kernel use $\rightarrow$ **poor FLOPS vs memory access**.

TRiSK-DG:



‘Staggered’ Discontinuous-Galerkin:

- Operate on DoF via ‘dense’ matrix-vector, matrix-matrix op’s.
- Efficient blockwise memory access patterns.
- Use BLAS/CUDA-style kernels $\rightarrow$ **improved FLOPS vs memory access**.

Sea-level rise and non-Boussinesq effects

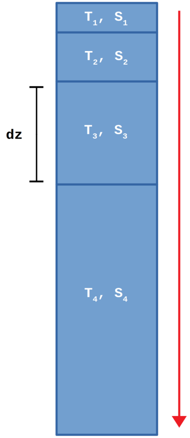
In addition to numerical improvements to the MPAS-O dycore, enhanced physics (equations-of-motion) are also targeted:

- Implement a non-Boussinesq (mass-conserving) formulation, to capture nonlinear sea-level height effects.
- (Lon-term) will facilitate tighter coupling with other cryosphere components (full 'mass-conserving' Earth system).
- Enhanced regional/coastal sea-level rise capabilities.

Boussinesq column (volume conservation)

Current volume-conserving (Boussinesq) formulation **does not account for 'steric'** contributions to sea-level rise:

'Volume' column:



Depth $\rightarrow$ pressures:

$$\frac{\partial p}{\partial z} = -g\rho(T, S, p_0)$$

Steric sea-level rise is a nonlinear thermodynamic interaction:

$$\mathrm{T}, \mathrm{S} \rightarrow \rho(T, S, p) \rightarrow \mathrm{SSH}$$

What happens to SSH in the **Boussinesq** model, given $\mathrm{T} + \delta\mathrm{T}$, $\mathrm{S} + \delta\mathrm{S}$

- Nothing...
- Since volume is conserved, $\delta\mathrm{T}$, $\delta\mathrm{S}$ do not perturb SSH.
- Such changes affect layer pressures instead.
- Physically, a Boussinesq model does not account for thermal-expansion / salinity-effects on SLR.

(T = temperature; S = salinity).

Non-Boussinesq column (mass conservation)

Need a new mass-conserving (non-Boussinesq) formulation **to account for 'steric'** contributions to sea-level rise:

Steric sea-level rise is a nonlinear thermodynamic interaction:

$$\mathrm{T}, \mathrm{S} \rightarrow \rho(T, S, p) \rightarrow \mathrm{SSH}$$

What about SSH in the **non-Boussinesq** model, given $\mathrm{T} + \delta\mathrm{T}$, $\mathrm{S} + \delta\mathrm{S}$

- Do get an SSH perturbation!
- Conserve mass (not volume), so $\delta\mathrm{T}$, $\delta\mathrm{S}$ perturbs SSH directly.
- Exchange role of z and p in equations-of-motion.
- Physically, a non-Boussinesq model **does** account for thermal-expansion / salinity-effects on SLR.

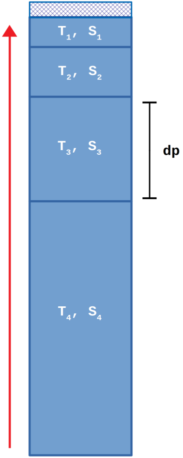
(T = temperature; S = salinity).

Pressure → depths:

$$\frac{\partial \Phi}{\partial p} = \rho^{-1}(T, S, p)$$

$$\Phi = gz$$

'Mass' column:



Outlook for MPAS-O:

Expect that future MPAS-O configurations will employ (even more) **'aggressive' variable resolution configurations + dynamic coupling**:

- Will place pressure on accuracy / robustness of existing TRiSK discretisation.
- Current formulation is limited to $\leq$ 1st-order convergence in certain cases.
- 'Modified' TRiSK (Calandrini et al) offers near-term opportunities to improve existing scheme (new weights, reconstructions, etc).
- Attempt a full dycore 'upgrade' over the longer-term: seek $\geq$ 2nd-order accuracy via advanced discretisation, scaling onto next-gen. architectures via dense kernels, etc.
- Solve the non-Boussinesq equations (mass-conservation) to enable nonlinear (regional) sea-level rise capabilities.