

Goal-oriented mesh adaptation for Firedrake

PI: Matt Piggott

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- 1. Extend PETSc's metric-based mesh adaptation functionality.
- 2. Pipe PETSc's mesh adaptation functionality through to Firedrake.
- 3. Develop a new goal-oriented error estimation and mesh adaptation module, Pyroteus.
- 4. Applications and documentation.



Metric-based mesh adaptation package. Written in C.

Solver library (amongst much more!). Written in C.



Finite element library. Written in Python, with automatic C code generation.



Goal-oriented error estimation module. Written in Python.

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1. Metric-based mesh adaptation in PETSc and Firedrake

Riemannian metric fields

An *nD* Riemannian metric, $\mathcal{M} = \{\underline{M}(x)\}_{x \in \Omega}$, takes the value of an $n \times n$ symmetric positive-definite (SPD) matrix at each point.

The space-time of general relativity

Riemannian metric fields



An *nD* Riemannian metric, $\mathcal{M} = \{\underline{M}(x)\}_{x \in \Omega}$, takes the value of an $n \times n$ symmetric positive-definite (SPD) matrix at each point.

Symmetry implies $\underline{M}(x) = \underline{V}(x)\underline{\Lambda}(x)\underline{V}^{T}(x),$

where

$$\underline{\Lambda}(\mathbf{x}) = \operatorname{diag}(\lambda_1(\mathbf{x}), \dots, \lambda_n(\mathbf{x})),$$

$$\underline{V}(\mathbf{x}) = [\mathbf{v}_1(\mathbf{x}) \dots \mathbf{v}_n(\mathbf{x})].$$

Positive-definiteness implies $\lambda_i > 0, \forall i = 1: n.$

Define
$$h_i \coloneqq \frac{1}{\sqrt{\lambda_i}}$$
, $\forall i = 1: n$.

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2D metric-based mesh adaptation



Minimise a quality function,

$$Q_{\mathcal{M}}(K) = \frac{\sqrt{3}}{2} \frac{\sum_{\gamma \in \partial K} \ell_{\mathcal{M}}(\gamma)^2}{|K|_{\mathcal{M}}}$$

for each mesh element *K*, by applying mesh modification operations.

Here $Q_{\mathcal{M}}(K)$ is minimised if K is an equilateral triangle with unit edges.

3D metric-based mesh adaptation



Minimise a quality function,

$$Q_{\mathcal{M}}(K) = \frac{\sqrt{3}}{216} \frac{\left(\sum_{\gamma \in \partial K} \ell_{\mathcal{M}}(\gamma)^2\right)^{\frac{3}{2}}}{|K|_{\mathcal{M}}}$$

for each mesh element *K*, by applying mesh modification operations.

Here $Q_{\mathcal{M}}(K)$ is minimised if K is a regular tetrahedron with unit edges.

Creating metric fields in PETSc

DMPlexMetricCreate DMPlexMetricCreateIsotropic DMPlexMetricCreateUniform DMPlexComputeGradientClementInterpolant

DMPlexMetricEnforceSPD DMPlexMetricSetMinimumMagnitude DMPlexMetricSetMaximumMagnitude DMPlexMetricSetMaximumAnisotropy DMPlexMetricSetTargetComplexity DMPlexMetricSetNormalizationOrder DMPlexMetricSetGradationFactor DMPlexMetricSetHausdorffNumber

DMPlexMetricAverage DMPlexMetricIntersection Isotropic metrics can be constructed easily:

$$\mathcal{M} = \varepsilon I.$$

A common choice of anisotropic metric is to use the Hessian of a field of interest, *u*:

$$\underline{H}(u) = \underline{V} \Lambda \underline{V}^T.$$

There are bounds on the interpolation error in u involving the Hessian.

Processing metric fields in PETSc

DMPlexMetricCreate DMPlexMetricCreateIsotropic DMPlexMetricCreateUniform DMPlexComputeGradientClementInterpolant

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DMPlexMetricAverage DMPlexMetricIntersection To make sure we have a metric, Hessians should be made SPD:

 $|\underline{H}| = \underline{V} |\underline{\Lambda}| \underline{V}^T.$

We can (approximately) enforce minimum/maximum element sizes by modifying $\underline{\Lambda}$.

It is usually a good idea to normalise the metric, too.



Combining metric fields in PETSc

DMPlexMetricCreate DMPlexMetricCreateIsotropic DMPlexMetricCreateUniform DMPlexComputeGradientClementInterpolant

DMPlexMetricEnforceSPD DMPlexMetricSetMinimumMagnitude DMPlexMetricSetMaximumMagnitude DMPlexMetricSetMaximumAnisotropy DMPlexMetricSetTargetComplexity DMPlexMetricSetNormalizationOrder DMPlexMetricSetGradationFactor DMPlexMetricSetHausdorffNumber

DMPlexMetricAverage DMPlexMetricIntersection Often there are multiple metrics that we want to take account of.

Metric averaging: mathematically simple, but not geometrically intuitive.

Metric intersection: geometrically intuitive, but not mathematically simple.



Using metric utilities in petsc4py

DMPlexMetricCreate DMPlexMetricCreateIsotropic DMPlexMetricCreateUniform DMPlexComputeGradientClementInterpolant

DMPlexMetricEnforceSPD DMPlexMetricSetMinimumMagnitude DMPlexMetricSetMaximumMagnitude DMPlexMetricSetMaximumAnisotropy DMPlexMetricSetTargetComplexity DMPlexMetricSetNormalizationOrder DMPlexMetricSetGradationFactor DMPlexMetricSetGradationFactor DMPlexMetricSetHausdorffNumber

DMPlexMetricAverage DMPlexMetricIntersection plex.metricCreate
plex.metricCreateIsotropic
plex.metricCreateUniform
plex.computeGradientClementInterpolant

plex.metricEnforceSPD
plex.metricSetMinimumMagnitude
plex.metricSetMaximumMagnitude
plex.metricSetMaximumAnisotropy
plex.metricSetTargetComplexity
plex.metricSetNormalizationOrder
plex.metricSetGradationFactor
plex.metricSetHausdorffNumber

plex.metricAverage
plex.metricIntersection

Metric fields in Firedrake

Proposed implementation gathers petsc4py metric utilities in a Riemannian metric class.

The underlying field data can be accessed and modified on either the Firedrake level (Function) or PETSc level (Vec). class RiemannianMetric(Metric): def set_parameters(self, **kwargs): def enforce_spd(self, **kwargs): ... def normalise(self, **kwargs): def average(self, *metrics): ... def intersect(self, *metrics): ...



Poisson test case in PETSc



 $\Delta x \approx (\text{element count})^{-3}$

Consider the Poisson problem $\Delta u = f$

on the unit cube with Dirichlet conditions.

We can manufacture an analytical solution by choosing f appropriately.

Example 1:
$$u(x, y, z) = \frac{4}{3}(x^2 + y^2 + z^2).$$

Poisson test case in PETSc



Consider the Poisson problem $\Delta u = f$

on the unit cube with Dirichlet conditions.

We can manufacture an analytical solution by choosing f appropriately.

Example 2: (smoothed) spherical indicator function.

 $\Delta x \approx (\text{element count})^{-\frac{1}{3}}$

Poisson test case in Firedrake

 $\Delta x \approx (\text{element count})^{-\frac{1}{3}}$





PETSc's mesh-to-mesh interpolation functionality does not currently work in parallel. Firedrake is similarly limited.



Source mesh

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Source mesh

1. Metric-based mesh adaptation: Summary of achievements

- Coupled Mmg and ParMmg mesh adaptation tools to PETSc.
- Implemented routines for creating, modifying and combining Riemannian metrics in PETSc, plus Python bindings.
- Added new PETSc tests and tutorials.
- Open pull request for piping functionality from PETSc to Firedrake.
 - Proposed RiemannianMetric class.
 - Basic tests of functionality.
- Open merge request for parallel mesh-to-mesh interpolation in PETSc.
 - Basic tests of functionality.

2. Goal-oriented error estimation and mesh adaptation using Pyroteus

Variational form:

$$a(u,v) = L(v), \quad \forall v \in V.$$

Weak form:

$$a(u_h, v) = L(v), \quad \forall v \in V_h \subset V.$$

Weak residual:

$$\rho(u_h, v) = L(v) - a(u_h, v), \qquad v \in V.$$

Variational form:

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Weak form:

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Weak residual:

$$\rho(u_h, v) = L(v) - a(u_h, v), \qquad v \in V.$$

Adjoint in variational form:

$$a(v, u^*) = J(v), \quad \forall v \in V.$$

Adjoint weak form:

$$a(v, u_h^*) = J(v), \quad \forall v \in V_h.$$

Variational form:

$$a(u, v) = L(v), \quad \forall v \in V.$$

Weak form:

$$a(u_h, v) = L(v), \quad \forall v \in V_h \subset V.$$

Weak residual:

$$\rho(u_h, v) = L(v) - a(u_h, v), \qquad v \in V.$$

Adjoint in variational form:

$$a(v, u^*) = J(v), \quad \forall v \in V.$$

Adjoint weak form:

$$a(v, u_h^*) = J(v), \quad \forall v \in V_h.$$

Dual weighted residual:

$$J(u) - J(u_h) \approx \rho(u_h, u^* - u_h^*).$$

Main difficulties:

- The true adjoint solution is generally unknown.
- We need to approximate it, e.g. by solving the adjoint problem again in an enriched finite element space.
- For time-dependent problems, we need to be able to solve both forward and adjoint problems across sequences of meshes.



Pyroteus goal-oriented error estimation toolkit

To tackle the time-dependent adaptation problem, we make use of a "mesh sequence", MeshSeq. The user just needs to provide:

TimePartition object

list of meshes

get_function_spaces(mesh)

get_form(mesh_seq)

get_solver(mesh_seq)

get_initial_condition(mesh_seq)

2. Goal-oriented error estimation and mesh adaptation using Pyroteus: Summary of achievements

Provided this information and a get_qoi(mesh_seq) function, the GoalOrientedMeshSeq subclass allows us to:

- Solve the forward problem over all meshes.
- Solve the adjoint problem over all meshes.
- Solve the adjoint problem over all "enriched" meshes.
- Compute goal-oriented error estimators based on this information.
- Perform goal-oriented mesh adaptation in a "fixed point iteration" type approach.



3. Applications and documentation

2D steady-state tracer transport test case



"Anisotropic DWR"



"Weighted Hessian"



"Weighted gradient"



Consider the advection-diffusion problem $\mathbf{u} \cdot \nabla c - \nabla \cdot (D\nabla c) = f, \quad c \in P1$

in a rectangular domain, where *f* is a point source. QoI: tracer concentration *c* in "receiver region".



2D steady-state tracer transport test case Analytical Isotropic DWR Weighted Hessian Uniform Anisotropic DWR Weighted gradient Hessian-based 0.20° 0.100Quantity of interest Quantity of interest 0.0750.150.050 0.10^{-10} 0.0250.050.000 10^{3} 10^{5} 10^{6} 10^{3} 10^{5} 10^{4} 10^{4} 10^{6} DoF count DoF count

3D steady-state tracer transport test case





Consider the same advection-diffusion problem

$$\mathbf{u} \cdot \nabla c - \nabla \cdot (D\nabla c) = f, \qquad c \in P1,$$

but extended to 3D in a cuboid domain. Again, QoI: tracer concentration *c* in "receiver region".





2D time-dependent desalination test case








	$t/T_{\rm tide}$	Elements	Vertices	Mean AR	Max. AR
	0.0	2,482	1,180	1.2	1.6
<	0.5	10,598	5,346	1.3	1.7
	1.0	12,500	6,304	1.2	1.7
2	1.5	12,104	6,099	1.3	3.0
\geq	2.0	2,278	1,180	1.3	3.0

(a) t = 0



(b) $t = 0.5 T_{\text{tide}}$

(c) $t = 1.5 T_{\text{tide}}$



(d) $t = T_{\text{tide}}$





~	$t/T_{\rm tide}$	Elements	Vertices	Mean AR	Max. AR
2	0.0	5,792	2,942	2.2	5.8
~	0.5	11,556	5,862	2.9	23.5
	1.0	12,555	6,365	2.3	13.0
2	1.5	10,231	5,191	2.3	18.9
K	2.0	4,931	2,515	1.7	5.4

(a) t = 0 s



(b) $t = 0.5 T_{\text{tide}}$

(c) $t = 1.5 T_{\text{tide}}$



(d) $t = T_{\text{tide}}$





Coll N	$t/T_{\rm tide}$	Elements	Vertices	Mean AR	Max. AR
1	0.0	2,426	1,254	2.7	11.3
24	0.5	12,473	6,280	1.8	11.1
N VIII	1.0	12,243	6,169	2.1	14.0
	1.5	13,523	6,809	2.0	17.7
144	2.0	2,708	1,395	1.5	3.3

(a) t = 0 s



(b) $t = 0.5 T_{\text{tide}}$

(c) $t = 1.5 T_{\text{tide}}$



(d) $t = T_{\text{tide}}$





$t/T_{\rm tide}$	Elements	Vertices	Mean AR	Max. AR
0.0	4,794	2,438	1.8	4.8
0.5	13,755	6,947	2.1	19.8
1.0	10,826	5,474	1.8	7.0
1.5	11,560	5,839	1.8	13.4
2.0	4,077	2,081	1.6	3.7

(a) t = 0 s



(b) $t = 0.5 T_{\text{tide}}$

(c) $t = 1.5 T_{\text{tide}}$



(d) $t = T_{\text{tide}}$





- Nonlinear shallow water equations. Solved for velocity and free surface elevation.
- Qol: energy output of tidal farm.
- $P1_{DG} P1_{DG}$ spatial discretisation with Roe fluxes, interior penalty method and Lax-Friedrichs stabilisation.
- Crank-Nicolson timestepping.









 $t=T_{\rm tide} - 16{,}553~{\rm elements} - 148{,}977~{\rm DoFs} - {\rm max}.$ aspect
 ratio2.2



 $t = 1.125\,T_{\rm tide}$ 47,392 elements 426,528 DoFs max. aspect ratio 2.3



 $t=1.25\,T_{\rm tide}$ 49,562 elements 446,058 DoFs max. aspect ratio 2.4



 $t = 1.375 T_{\text{tide}}$ 8,307 elements 74,763 DoFs max. aspect ratio 2.1



 $t = 1.5 T_{\text{tide}}$ 8,282 elements 74,538 DoFs max. aspect ratio 2.4

Isotropic adaptation





Velocity Magnitude (m/s) 0.0 0.5 1 1.5 2 2.5 3 3.5 4.0



 $t=T_{\rm tide} ~~35,\!381$ elements $~318,\!429$ DoFs $~~{\rm max.}$ aspect ratio 8.3



 $t = 1.125\,T_{\rm tide}$ 27,772 elements 249,948 DoFs max. a
spect ratio 10.4



 $t = 1.25 T_{\text{tide}}$ 23,503 elements 211,527 DoFs max. aspect ratio 21.8



 $t=1.375\,T_{\rm tide}$ ~27,475 elements ~247,275 DoFs ~ max. aspect ratio 26.2



 $t=1.5\,T_{\rm tide}$ 13,482 elements 121,338 DoFs max. aspect ratio 5.8

Anisotropic adaptation



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Staggered		
(uniform)	Configuration	R
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Configuration	Run	\mathcal{C}^1	\mathcal{C}^2	\mathcal{C}^3	\mathcal{C}^4	\mathcal{C}^5	\mathcal{F}
Aligned	Uniform mesh Isotropic Anisotropic	$2.75 \\ 2.73 \\ 2.72$	$0.82 \\ 0.79 \\ 0.80$	$1.76 \\ 1.39 \\ 1.51$	$1.27 \\ 1.52 \\ 1.58$	$1.48 \\ 1.52 \\ 1.46$	8.07 7.93 8.07
Staggered	Uniform mesh Isotropic Anisotropic	$3.07 \\ 3.06 \\ 3.06$	$3.61 \\ 3.54 \\ 3.57$	$2.49 \\ 2.23 \\ 2.27$	$2.47 \\ 2.19 \\ 2.15$	$2.98 \\ 2.30 \\ 2.25$	$14.62 \\ 13.33 \\ 13.30$

mparison

Configuration	Run	\mathcal{C}^1	\mathcal{C}^2	\mathcal{C}^3	\mathcal{C}^4	\mathcal{C}^5	\mathcal{F}
Aligned	Iso. — Fixed Aniso. — Fixed Iso. — Aniso.	-0.9% -1.2% 0.3%	-4.1% -2.1% -2.0%	-21.1% -13.9% -7.3%	$19.7\% \\ 24.5\% \\ -4.8\%$	2.9% -1.1% 4.0%	-1.7% -0.0% -1.7%
Staggered	Iso. — Fixed Aniso. — Fixed Iso. — Aniso.	-0.2% -0.1% -0.1%	-1.8% -1.0% -0.8%	-10.7% -9.1% -1.6%	-11.3% -13.2% 2.0%	-22.6% -24.5% 2.0%	-8.8% -9.0% 0.2%

Relative differences in energy output



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Staggered (uniform)	Configuration
	Aligned
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Staggered (isotropic)	Staggered
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M M	Configuration
Staggered (anisotropic)	Aligned
	Staggered
AND TO THE A	Relative dif

Configuration	Run	\mathcal{C}^1	\mathcal{C}^2	\mathcal{C}^3	\mathcal{C}^4	\mathcal{C}^5	${\cal F}$
Aligned	Uniform mesh Isotropic Anisotropic	$2.75 \\ 2.73 \\ 2.72$	$0.82 \\ 0.79 \\ 0.80$	$1.76 \\ 1.39 \\ 1.51$	$1.27 \\ 1.52 \\ 1.58$	$1.48 \\ 1.52 \\ 1.46$	8.07 7.93 8.07
Staggered	Uniform mesh Isotropic Anisotropic	$3.07 \\ 3.06 \\ 3.06$	$3.61 \\ 3.54 \\ 3.57$	$2.49 \\ 2.23 \\ 2.27$	$2.47 \\ 2.19 \\ 2.15$	$2.98 \\ 2.30 \\ 2.25$	$14.62 \\ 13.33 \\ 13.30$

put comparison

Configuration	Run	\mathcal{C}^1	\mathcal{C}^2	\mathcal{C}^3	\mathcal{C}^4	\mathcal{C}^5	${\cal F}$
Aligned	Iso. — Fixed Aniso. — Fixed Iso. — Aniso.	-0.9% -1.2% 0.3%	-4.1% -2.1% -2.0%	-21.1% -13.9% -7.3%	$19.7\% \\ 24.5\% \\ -4.8\%$	2.9% -1.1% 4.0%	-1.7% -0.0% -1.7%
Staggered	Iso. — Fixed Aniso. — Fixed Iso. — Aniso.	-0.2% -0.1% -0.1%	-1.8% -1.0% -0.8%	-10.7% -9.1% -1.6%	-11.3% -13.2% 2.0%	-22.6% -24.5% 2.0%	-8.8% -9.0% 0.2%

fferences in energy output



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Metric-based mesh adaptation

DMPlex supports mesh adaptation using the *Riemmanian metric framework*. The idea is to use a Riemannian metric space within the mesher. The metric space dictates how mesh resolution should be distributed across the domain. Using this information, the remesher transforms the mesh such that it is a *unit mesh* when viewed in the metric space. That is, the image of each of its elements under the mapping from Euclidean space into the metric space has edges of unit length.

One of the main advantages of metric-based mesh adaptation is that it allows for fully anisotropic remeshing. That is, it provides a means of controlling the shape and orientation of elements in the adapted mesh, as well as their size. This can be particularly useful for advectiondominated and directionally-dependent problems.

See [Ala10] for further details on metric-based anisotropic mesh adaptation.

The two main ingredients for metric-based mesh adaptation are an input mesh (i.e. the DMPlex) and a Riemannian metric. The implementation in PETSc assumes that the metric is piecewise linear and continuous across elemental boundaries. Such an object can be created using the routine

DMPlexMetricCreate(DM dm, PetscInt f, Vec *metric);

A metric must be symmetric positive-definite, so that distances may be properly defined. This



Accessing the PETSc mesh representation

Under the hood, Firedrake uses PETSc's DMPlex unstructured mesh representation. It uses a hierarchical approach, where entities of different dimension are put on different levels of the hierarchy. The single tetrahedral element shown on the left below may be interpreted using the graph representation on the right. Entities of dimension zero (vertices) are shown at the top. Entities of dimension one (edges) are shown on the next level down. Entities of dimension two (faces) are shown on the penultimate level and the (dimension three) element itself is on the bottom level. Edges in the graph indicate which entities own/are owned by others.



The DMPlex associated with a given mesh may be accessed via its topology_dm attribute:

plex = mesh.topology_dm

All entities in a DMPlex are given a unique number. The range of these numbers may be deduced using the method plex.getDepthStratum, whose only argument is the entity dimension sought. For example, 0 for vertices, 1 for edges, etc. Similarly, the method plex.getHeightStratum can be used for codimension access. For example, height 0 corresponds to cells. The hierarchical DMPlex structure may be traversed using other methods, such as plex.getCone, plex.getSupport and plex.getTransitiveClosure. See the Firedrake DMPlex paper and the PETSc manual for details.

If vertex coordinate information is to be accessed from the DMPlex then we must first establish a mapping between its numbering and the coordinates in the Firedrake mesh. This is done by establishing a 'section'. A section provides a way of associating data with the mesh - in this case,

firedrakeproject.org

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Pyroteus manual

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Pyroteus Goal-Oriented Mesh Adaptation Toolkit

Pyroteus provides metric-based goal-oriented mesh adaptation functionality to the Python-based finite element library Firedrake. The 'y' is silent, so its pronunciation is identical to 'Proteus' - the ancient Greek god of the constantly changing surface of the sea.

Mathematical background

Goal-oriented mesh adaptation presents one of the clearest examples of the intersection between adjoint methods and mesh adaptation. It is an advanced topic, so it is highly recommended that users are familiar with adjoint methods, mesh adaptation and the goal-oriented framework before starting with Pyroteus.

We refer to the Firedrake documentation for an introduction to the finite element method - the discretisation approach assumed throughout. The *dolfin-adjoint* package (which Pyroteus uses to solve adjoint problems) contains some excellent documentation on the mathematical background of adjoint problems. The goal-oriented error estimation and metric-based mesh adaptation functionalities provided by Pyroteus are described in the manual.

- Pyroteus manual
 - 1. Motivation
 - 2. Goal-oriented error estimation
 - 3. The metric-based framework
 - 4. Goal-oriented mesh adaptation

API documentation

The classes and functions which comprise Pyroteus may be found in the API documentation.

pyroteus.github.io

3. Applications and documentation: Summary of achievements

- Tested functionality in two research papers.

- Metric-based mesh adaptation section in the PETSc manual.
- Extension of existing Firedrake documentation.
- Created a webpage for Pyroteus: <u>pyroteus.github.io</u>, including plenty of documentation and demos.

Papers

About eCSE work

- <u>JGW</u>, M. G. Knepley, N. Barral, M. D. Piggott, *Parallel metric-based mesh adaptation in PETSc using ParMmg*, 30th International Meshing Roundtable (2022), doi:<u>10.48550/arXiv.2201.02806</u>.
- <u>JGW</u>, A. K. Mohan, M. D. Piggott, *Pyroteus Goal-Oriented Error Estimation Toolkit*, 31st
 International Meshing Roundtable (in preparation).

Using eCSE work

- <u>JGW</u>, N. Barral, D. A. Ham, M. D. Piggott, Goal-oriented error estimation and mesh adaptation for tracer transport modelling, Computer-Aided Design 145 (2022): 103187, doi:<u>10.1016/j.cad.2021.103187.</u>
- <u>JGW</u>, A. Angeloudis, N. Barral, L. Mackie, S. C. Kramer, M. D. Piggott, *Tidal array* modelling using goal-oriented mesh adaptation, Journal of Ocean Engineering and Marine Energy (under review), doi:<u>10.31223/X5H06B</u>.

Thanks for listening!