Optimal transport and mesh generation on the plane and the sphere

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PDE computations often need to use a computational mesh which can

- Capture small scales
- Is aligned with the solution
- Resolve local geometry eg. orography

This is needed

- For accurate numerical computation of anisotropic evolving features eg. storms, fronts possibly on the sphere
- For accurate approximation of anisotropic functions on many scales eg. For data assimilation calculations

Eady Equations

Front formation for the Eady Equations of a tropical storm



- Want to construct a suitable mesh τ : Various methods eg. mesh refinement, mesh relocation
- *r*-adaptivity: <u>relocate</u> mesh vertices, preserving mesh connectivity/topology.
- When done dynamically, <u>"moving mesh" method</u>.
- Some advantages over *h*-adaptive refinement
 - Can avoid sudden changes in mesh resolution
 - Control over global mesh regularity
 - $\bullet\,$ Mesh topology unchanged $\,\Longrightarrow\,$ constant data structures
 - Avoids the obvious load-balance issue when used in parallel

Video: Moving a mesh on the sphere

- Some disadvantages:
 - Solution of an extra PDE adds complexity and computational cost
 - Unchanging topology constrains refinement at a global scale
 - Can give rise to skew meshes
 - Poor algorithm can lead to tangling



Mesh density controlled by monitor function $m(\vec{x}) > 0$, through equidistribution:

 $m(x) \times \text{cell area} = \text{const}$

(or $\int_{\text{cell}} m \, \mathrm{d}\vec{x} = \text{const}$).

In practice, m will be derived from current simulation state of solution u(x), e.g.

- $m \propto \|\nabla u\|^p$, $\|\nabla \nabla u\|^p$, etc., so that 'the function u(x) is represented as well as possible' (minimise interpolation error)
- m based on diagnostic derived from physical principles, e.g. vorticity
- Estimates of local interpolation or truncation error

Notation:

- Ω_C "computational" domain eg. plane, sphere (often with uniform mesh)
- Ω_P "physical" domain
- $\vec{\xi}$ coordinate in computational domain
- \vec{x} coordinate in physical domain







Adapted mesh is defined by a map $\vec{x}(\vec{\xi})$

The Jacobian of this map is J, $J_{ij} := \frac{\partial x_i}{\partial \xi_i}$

Equidistribution requirement:

$$m(\vec{x}) \det J = \text{const} =: \theta$$

Equidistribution requirement:

 $m(\vec{x}) \det J = \theta$

In 1D, this defines the mesh (almost) uniquely. In 2D/3D, additional regularisation constraints are needed. Budd & Williams (2006): subject to (1), pick $\vec{x}(\vec{\xi})$ minimising

$$\int_{\Omega_C} |\vec{x}(\vec{\xi}) - \vec{\xi}|^2 \,\mathrm{d}\vec{\xi}.$$

Prevents tangling and reduces skewness.

(1)

OT-based mesh generation on the plane

Well-known result from Optimal Transport literature (Brenier, 1991):

There exists a unique map $\vec{x}(\vec{\xi})$ that minimises

$$\int_{\Omega_C} |\vec{x}(\vec{\xi}) - \vec{\xi}|^2 \,\mathrm{d}\vec{\xi}$$

subject to the requirement $m(\vec{x}) \det J = \theta$. Furthermore, this can be written as the gradient of a convex 'potential' function, $\tilde{\phi}(\vec{\xi})$:

$$\vec{x} =
abla_{\xi} \tilde{\phi}.$$

Note: convex \implies no tangling!

We will actually write

$$\vec{x} = \vec{\xi} + \nabla_{\xi}\phi$$
 $(\phi \approx \tilde{\phi} - \frac{1}{2}|\xi|^2)$

Better for periodic domains, and generalises to the Sphere

OT-based mesh generation on the plane

Substituting $\vec{x} = \vec{\xi} + \nabla \phi$ into the definition of J gives

 $J = I + \nabla \nabla \phi.$

The governing equation is then

 $m(\vec{x})\det(I+\nabla\nabla\phi)=\theta.$

In 2D plane, this is a Monge-Ampère equation

 $m(\vec{x})((1 + \phi_{xx})(1 + \phi_{yy}) - \phi_{xy}^2) = \theta.$

Couple to Neumann or periodic boundary conditions

- Fully nonlinear product of second derivatives of ϕ
- $m(\vec{x})$ is a function of $\nabla \phi$

OT-based mesh generation on the sphere S_2

We use the same approach on the sphere S_2 : pick $\vec{x}(\vec{\xi}) : S_2 \to S_2$ minimising

 $\int_{\Omega_C} \|\vec{x}(\vec{\xi}) - \vec{\xi}\|^2 \,\mathrm{d}\vec{\xi},$

where $\|\cdot\|$ is now *geodesic* distance, subject to the equidistribution requirement $m(\vec{x}) \det J = \theta$.

McCann (2001) For a general manifold \mathcal{M} there is a unique such map $\vec{x}(\vec{\xi})$, and there exists a scalar function $\phi(\vec{\xi}) : \mathcal{M} \to R$, $\nabla \phi \in T_{\xi}\mathcal{M}$:

 $\vec{x} = \exp(\nabla \phi) \vec{\xi}.$

OT-based mesh generation on the sphere

Intuitively, the **exponential map** $\vec{x} = \exp(\nabla \phi) \vec{\xi}$ is:

- Start at $\vec{\xi}$
- ${\it @}$ Travel along geodesic in direction of $\nabla\phi$
- Stop after distance $|
 abla \phi|$
- On plane, $\exp(\nabla \phi)\vec{\xi} = \vec{\xi} + \nabla \phi$
- On sphere with radius R centred at the origin, Rodrigues' map gives

$$\exp(\nabla\phi) \vec{\xi} = \cos\left(\frac{|\nabla\phi|}{R}\right) \vec{\xi} + R\sin\left(\frac{|\nabla\phi|}{R}\right) \frac{\nabla\phi}{|\nabla\phi|}$$

OT-based mesh generation on the sphere



Now write equidistribution equation $m(\vec{x}) \det J = \theta$ in terms of $\phi(\xi)$

We treat $\vec{x}(\vec{\xi})$ as a map from \mathbb{R}^3 to \mathbb{R}^3 (partly for software reasons).

J is then rank-deficient. We produce an "equivalent" object of full rank, giving the **Monge-Ampere-like equation**

 $m(\vec{x}) \det((\nabla \exp(\nabla \phi)\vec{\xi}) \cdot P_{\xi} + \vec{k}_P \otimes \vec{k}_C) = \theta,$

where $P_{\xi} := I - \vec{k}_C \otimes \vec{k}_C$ is a projection matrix, \vec{k}_P and \vec{k}_C are unit normal vectors at \vec{x} and $\vec{\xi}$, and the earlier formula is used for the exponential map.

Analogous to adding $(0,0,1)\otimes(0,0,1)$ to a 2x2 matrix to produce an "equivalent" 3x3 matrix.

Numerical solution of MA on the plane

 $m(\vec{x})\det(I+\nabla\nabla\phi)=\theta.$

Mixed finite element approach, based on Lakkis and Pryer (2011, 2013): to get a stable method, introduce discrete variable σ representing $\nabla \nabla \phi$.

Let $\langle -, - \rangle$ denote the obvious inner product $\int_{\Omega_c} \cdot d\vec{\xi}$.

For suitable finite element spaces V_1 , V_2 , we seek $\phi \in V_1, \sigma \in V_2$ s.t.

$$egin{aligned} &\langle m{v}, m{m}(
abla \phi) \det(m{I} + \sigma)
angle &= \langle m{v}, heta
angle, \qquad orall m{v} \in m{V}_1 \ &\langle au, \sigma
angle + \langle
abla \cdot au,
abla \phi
angle &= 0, \qquad orall au \in m{V}_2. \end{aligned}$$

On triangles: $V_1 = P_2$ (continuous, piecewise-quadratic), $V_2 = P_2^{(2\times 2)}$ On quads: $V_1 = Q_2$ (continuous, piecewise-biquadratic), $V_2 = Q_2^{(2\times 2)}$ Seek $\phi \in V_1, \sigma \in V_2$ such that

$$\langle v, m(\nabla \phi) \det(I + \sigma) \rangle = \langle v, \theta \rangle, \quad \forall v \in V_1$$

$$\langle \tau, \sigma \rangle + \langle \nabla \cdot \tau, \nabla \phi \rangle = 0, \quad \forall \tau \in V_2.$$

$$(3)$$

We look at two ways of solving the nonlinear system (2)-(3):

- Relaxation method
- Quasi-Newton method

Given (ϕ^n, σ^n) , how to obtain $(\phi^{n+1}, \sigma^{n+1})$?

Iteration:

$$-\nabla^2 \phi^{n+1} = -\nabla^2 \phi^n + \Delta(m(\nabla \phi^n) \det(I + \nabla \nabla \phi^n) - \theta^n),$$

with Δ some 'step size'.

Full version based on Awanou (2015): **obtain** ϕ^{n+1} by solving $\langle \nabla v, \nabla \phi^{n+1} \rangle = \langle \nabla v, \nabla \phi^n \rangle + \Delta \langle v, m(\nabla \phi^n) \det(I + \sigma^n) - \theta^n \rangle, \quad \forall v \in V_1,$ then **obtain** σ^{n+1} by solving

 $\langle \tau, \sigma^{n+1} \rangle = -\langle \nabla \cdot \tau, \nabla \phi^{n+1} \rangle, \qquad \forall \tau \in V_2.$

This converges to the solution of the nonlinear problem if $\Delta \ll 1$

Unfortunately, we don't have a good a-priori estimate for 'optimal' Δ .

Given $\phi^n, \sigma^n \ldots$

• Use ϕ^n to evaluate the coordinates \vec{x} of Ω_P via L^2 -projection: $\vec{x}(\vec{\xi}) = \vec{\xi} + \prod_{[P_1/Q_1]^2} \nabla \phi^n(\vec{\xi}).$

2 Evaluate $m(\vec{x})$ at vertices of Ω_P (assuming analytic expression)

3 Evaluate
$$heta^n := \int_{\Omega_C} m \det(I + \sigma^n) \, \mathrm{d}x / \int_{\Omega_C} \, \mathrm{d}x$$

- **③** Solve Poisson problem to obtain ϕ^{n+1} (CG/GAMG)
- Solve mass matrix system to obtain σ^{n+1} (CG/ILU)
- Evaluate termination condition; stop if met.

Plane test cases

$$m(\vec{x}) = 1 + \alpha_1 \operatorname{sech}^2(\alpha_2(|\vec{x} - \vec{x_c}|^2 - a^2))$$

• Ring:
$$a = 0.25$$
, $\alpha_1 = 10$, $\alpha_2 = 200$

• Bell:
$$a = 0$$
, $\alpha_1 = 50$, $\alpha_2 = 100$



Final ring mesh:



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Delft, December, 2019 21 / 55

Convergence for ring test case, $\Delta=0.1$



Final bell mesh:



Convergence for bell test case, $\Delta = 0.04$



Nonlinear residual is

 $R \equiv \langle \tau, \sigma^n \rangle + \langle \nabla \cdot \tau, \nabla \phi^n \rangle - \langle \nu, m(\vec{x}) \det(I + \sigma^n) - \theta^n \rangle, \quad \forall \nu \in V_1, \tau \in V_2.$

Apply a **Newton method** to this.

Full Newton is problematic as Newton steps do not respect convexity

Newton method

Step 0:



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Newton method

Step 1:



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Nonlinear residual:]

 $R \equiv \langle \tau, \sigma^n \rangle + \langle \nabla \cdot \tau, \nabla \phi^n \rangle - \langle \nu, m(\vec{x}) \det(I + \sigma^n) - \theta^n \rangle, \quad \forall \nu \in V_1, \tau \in V_2.$

We instead use a **Quasi-Newton method**, with a Jacobian that ignores the dependence of m on ϕ . On the plane, this is

 $\begin{aligned} &\langle \tau, \delta \sigma \rangle + \langle \nabla \cdot \tau, \nabla \delta \phi \rangle \\ &- \langle v, m(\vec{x}) (\delta \sigma_{11} (1 + \sigma_{22}^n) + (1 + \sigma_{11}^n) \delta \sigma_{22} - \delta \sigma_{12} \sigma_{21}^n - \sigma_{12}^n \delta \sigma_{21} \rangle. \end{aligned}$

We omit the $-\langle v, \nabla \delta \phi \cdot \nabla m |_{\vec{x}} \det(I + \sigma^n) \rangle$ term.

Nonlinear solver: l^2 -minimisation line search quite robust but not perfect

Linear solver: Gory details:

- Preconditioned GMRES on outer system
- 'Riesz map' preconditioner $\langle v, \delta \phi \rangle_{H^1} + \langle \tau, \delta \sigma \rangle_{L^2}$, sufficient for (asymptotically) mesh-independent convergence.
- Outer preconditioner application: block Gauss-Seidel
- Inner solves: PETSc's GAMG for $\delta\phi$ block, ILU for $\delta\sigma$.

Both linear and nonlinear convergence appear to be independent of problem size.

Quasi-Newton method

Comparison of methods on ring test case



Quasi-Newton method

Comparison of methods on bell test case



Numerical solution on the sphere

Now solve the Monge-Ampere-like equation $m(\vec{x}) \det((\nabla \exp(\nabla \phi)\vec{\xi}) \cdot P_{\xi} + \vec{k}_P \otimes \vec{k}_C) = \theta,$

Discretise by adapting the mixed finite element methods on the plane. **Set**

 $\sigma = \nabla \exp(\nabla \phi) \vec{\xi}.$

The nonlinear discrete equations are then

$$egin{aligned} &\left\langle \mathbf{v}, \mathbf{m}(ec{\mathbf{x}}) \det \left(\sigma \cdot P_{\xi} + rac{\exp(
abla \phi) ec{\xi}}{R} \otimes rac{ec{\xi}}{R}
ight)
ight
angle &= \langle \mathbf{v}, heta
angle, & orall \mathbf{v} \in V_1, \ &\left\langle au, \sigma
angle + \langle
abla \cdot au, \exp(
abla \phi) ec{\xi}
ight
angle &= 0, & orall au \in V_2. \end{aligned}$$

Can solve using relaxation or quasi-Newton methods.

Sphere test cases: 1. Ringler monitor function

$$m(\vec{x}) = \sqrt{\frac{1-\gamma}{2}} \left(\tanh \frac{\beta - \|\vec{x} - \vec{x_c}\|}{\alpha} + 1 \right) + \gamma,$$

• $\alpha = \frac{\pi}{20}, \ \beta = \frac{\pi}{6}, \ \gamma = \left(\frac{1}{2}\right)^4, \left(\frac{1}{4}\right)^4, \left(\frac{1}{8}\right)^4, \left(\frac{1}{16}\right)^4$



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Sphere: Ringler

'Convergence' of relaxation method on a cubed-sphere mesh



We appear to only get convergence for very gentle monitor functions.

Canadian Breakthrough: use higher-order representation for \vec{x} and $\vec{\xi}$ (not ϕ and σ !)

E.g. one can mesh a sphere using 'flat' triangles. However, in this problem, we don't get convergence for a general monitor function unless each mesh cell is quadratic (or higher).

Similarly, on a quadrilateral mesh, need to use a biquadratic representation (or higher) rather than bilinear.

Sphere

Convergence of relaxation method on biquadratic cubed-sphere mesh



Sphere: Ringler and biquadratic cubed-sphere



Front/back of mesh, $\gamma = (1/8)^4$

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Sphere: 2. Cosine Bell monitor function



Bell shaped monitor function on an Icosahedral mesh

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Delft, December, 2019 38 / 55

Sphere: 3. Two ring monitor function



Monitor function concentrated in two rings on an icosahedral mesh

Mesh Regularity

- Mesh regularity follows from the regularity of the solutions of the Monge-Ampere equation and the optimal transport problem
- Studied on the sphere by McCann and Loeper
- Positive curvature of the sphere and lack of a boundary leads to Good Regularity of the MA solutions [Loeper] which is better than the regularity on the plane
- Local regularity of the mesh is related to its scale s and its skewness Q
- If J is the local linearisation of the map with eigenvalues λ_1, λ_2 then

$$s = \lambda_1 \lambda_2, \quad Q = \frac{1}{2} \left[\frac{\lambda_1}{\lambda_2} + \frac{\lambda_2}{\lambda_1} \right].$$

• Uniform mesh Q = 1, OT mesh, Q close to one.

Sphere: Skewness



Skewness Q of the Ringler monitor function generated mesh

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Implementation

Implemented using Firedrake (firedrakeproject.org): software for highly-automated solution of PDEs using FEM. Closely related to FEniCS

```
from firedrake import *
mesh = UnitCubedSphereMesh (refinement_level=4, degree=2)
V1 = FunctionSpace(mesh, "Q", 2)
V2 = TensorFunctionSpace(mesh, "Q", 2)
V = V1 * V2
phisigma = Function(V)
phi, sigma = split (phisigma)
xi = Function (mesh.coordinates)
theta = Constant(...)
m = ...
v, tau = TestFunctions(V)
modgphi = sqrt(dot(grad(phi), grad(phi)))
expxi = xi * cos(modgphi) + grad(phi) * sin(modgphi) / modgphi
projxi = Identity(3) - outer(xi, xi)
dot(sigma, proixi)) - theta)*v*dx
solve(F == 0, phisigma, solver_parameters={"ksp_type": "gmres",
                                       "pc_type" "fieldsplit".
                                       ...})
```

Implementation

```
static inline void form00_cell_integral_otherwise (double A[9][9], const double *const restrict
      *restrict coords , const double *const restrict *restrict w.0 , const double *const restrict
      *restrict w_1 . const double *const restrict *restrict w_2 . const double *const restrict *restrict
      w_3) {
  static const double t0[5][2] = \{\{0.953089922969332, 0.046910077030668\}, \dots \}
  for (int ip_0 = 0; ip_0 < 5; ip_0 += 1) {
    double t4 = (((w_1[2][2] * t2[ip_0][0]) + (w_1[5][2] * t2[ip_0][1])) + (w_1[8][2] * t2[ip_0][2]));
    for (int ip_1 = 0; ip_1 < 5; ip_1 += 1) {
      double t66 = ((t0[ip_1][0] * t65) + (t0[ip_1][1] * t64));
      for (int k0 = 0; k0 < 3; k0 += 1) {
        for (int k1 = 0; k1 < 3; k1 += 1) {
          t157[k0][k1] = (t2[ip_1][k1] * (((((((t3[ip_0][k0] * ct79) * ct169) + ((t3[ip_0][k0] * ct79)...))))))
       }
      }
      double t158 = ((t70 * t75) + (-1 * (t74 * t71)));
      for (int k0 = 0; k0 < 3; k0 += 1) {
       for (int k1 = 0; k1 < 3; k1 += 1) {
          ct362[k0][k1] = t157[k0][k1] * ct361;
       }
      }
      for (int j0 = 0; j0 < 3; j0 += 1) {
       for (int i1 = 0; i1 < 3; i1 += 1) {
          double t162 = (t2[ip_0][j0] * t2[ip_1][j1]);
          for (int k0 = 0; k0 < 3; k0 += 1) {
           for (int k1 = 0; k1 < 3; k1 += 1) {
             A[(i0 * 3) + i1][(k0 * 3) + k1] + t162 * ct362[k0][k1];
}
```

Extension: A faster method to generate the mesh

• Improve convergence of Newton solver by using something closer to full Newton.

E.g. add a small fourth-order term to loosen the convexity requirement (Feng & Neilan, 2009).

 $-\epsilon \nabla^4 \phi + m(\vec{x}) \det(I + \nabla \nabla \phi) = \theta$

Sacrifices true equidistribution, but gives much better linear and nonlinear performance.

Preliminary experiments, using FE discretisation of Brenner et al. (2011) for fourth-order term:

Extension: A faster method to generate the mesh

Ring



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Extension: A faster method to generate the mesh

Bell



Data assimilation

Eg Operational mesh calculation for meteorological data assimilation

Frontal system: Rain storm in SW UK



Data assimilation

Take m to be a scaled approximation of the Potential Vorticity of the 3D flow



Coupled to 1d DA procedure [Piccolo, Cullen, Browne]

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Solution of Monge-Ampere on the Sphere

Solving a PDE on the mesh

• Can couple the moving mesh approach to solve geophysical PDEs

Short term goal: Continuity and Shallow Water Equations.

Preliminary work on advection equation:

$$rac{\partial q}{\partial t} + (ec{u} \cdot
abla)q = 0$$

with scalar q and prescribed \vec{u} .

DG approach, SSPRK3 timestepping,

 $m \propto \|\nabla \nabla q\| + const$:

Solving equations on the moving mesh: Lagrangian approach

So, for the advection equation in the moving frame, mesh velocity \vec{v}

$$rac{\partial q}{\partial t} + ((ec{u} - ec{v}) \cdot
abla)q = 0,$$

we do

- $\frac{1}{2}\Delta t$ Eulerian continuity $(\vec{u} \vec{v})$ on old mesh
- Move mesh, and adjust values using $\langle \phi, q
 angle_{
 m new} = \langle \phi, q
 angle_{
 m old}$, $orall \phi \in V$
- $\frac{1}{2}\Delta t$ Eulerian continuity $(\vec{u} \vec{v})$ on new mesh

Buckley-Leverett

Eg Buckley-Leverett equation (gas dynamics)

$$u_t = -F_x - G_y + \mu \nabla^2 u, \quad F(u) = u^2 / (u^2 + (1-u)^2), \quad G(u) = (1-5(1-u)^2) F$$

Solve using simultaneous mesh and solution calculation with m the solution arc-length



Rezoning: Possibly a more practical method

- Can couple the moving mesh method to much standard software for solving a general time-dependent PDE
- At time level t_k advance the solution the PDE on the current mesh to give solution at time level t_{k+1}. Using a standard software package eg. Discontinuous Galerkin method, Finite element method, Finite volume method (OpenFoam)
- Using the new solution, calculate a new mesh at time level t_{k+1} using the Monge-Ampere based approach
- Interpolate the solution at time level t_{k+1} onto the new mesh.
- Take care to conserve mass (or other desired physical properties) where appropriate. Fine tune the mesh if needed
- Optional Repeat the mesh calculation if needed
- Repeat from the top

Eady Equations

Front formation for the Eady Equations of a tropical storm



- By design, we generate small cells, which restricts timestep through CFL for explicit methods (⇒ need to control *m* or use SISL methods or similar)
- Can get $\|\vec{u} \vec{v}\| \gg \|\vec{u}\|$ in artificial test problems, which restricts Δt further.
- However, Moving mesh can work in our favour in realistic problems we often get $\vec{v} \approx \vec{u}$ where small cells are present, as the resolution tracks the feature
- Post-processing of m smoothing to control Δx

Summary

- We produce 'optimally-transported' meshes on the plane and sphere
- By solving Monge-Ampere-type PDEs
- This uses a mixed finite element discretisation of the PDEs
- Relaxation approach bulletproof, but takes many iterations
- Quasi-Newton approach robust except for hard m
- Sphere requires higher-order mesh representation for convergence
- Parallel 'just works' (due to Firedrake).
- Coupling to PDEs works so far.

Hilary Weller, Phil Browne, B & Mike Cullen (2016), *Mesh adaptation on the sphere using optimal transport and the numerical solution of a Monge–Ampère type equation*, JCP

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