Optimal Transport Methods for Mesh Generation: With applications to Meteorology

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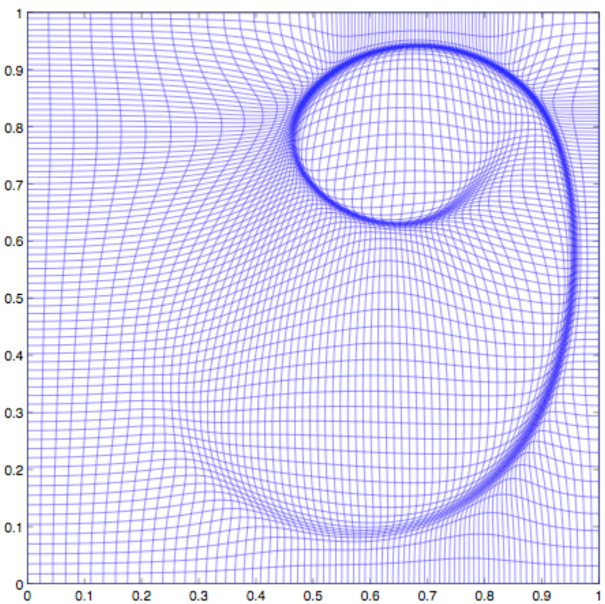


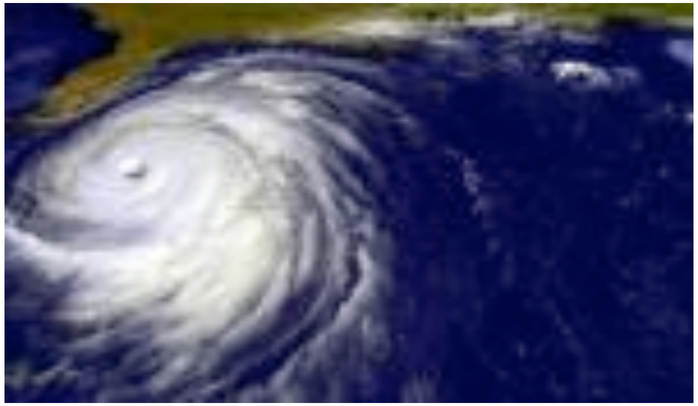
UNIVERSITY OF BATH

Kansas May 2013

In numerical weather prediction and other PDE based computations often need to locally refine a mesh to capture small scales

(i) To resolve local geometry eg. orography

(ii) For accurate numerical computation of evolving features eg. storms, fronts



(i) For accurate assimilation of observed data to avoid spurious correlations in data assimilation procedures r-adaptive moving mesh methods aim to do this by the 'optimal placement' of a fixed number of mesh points which move during the computation

There are many advantages with r-adaptivity

- Constant data structures and mesh topology
- Ease of coupling to CFD solvers and DA codes
- Capturing dynamical physics of the solution

eg. Lagrangian behaviour, symmetries, conservation laws, self-similarity

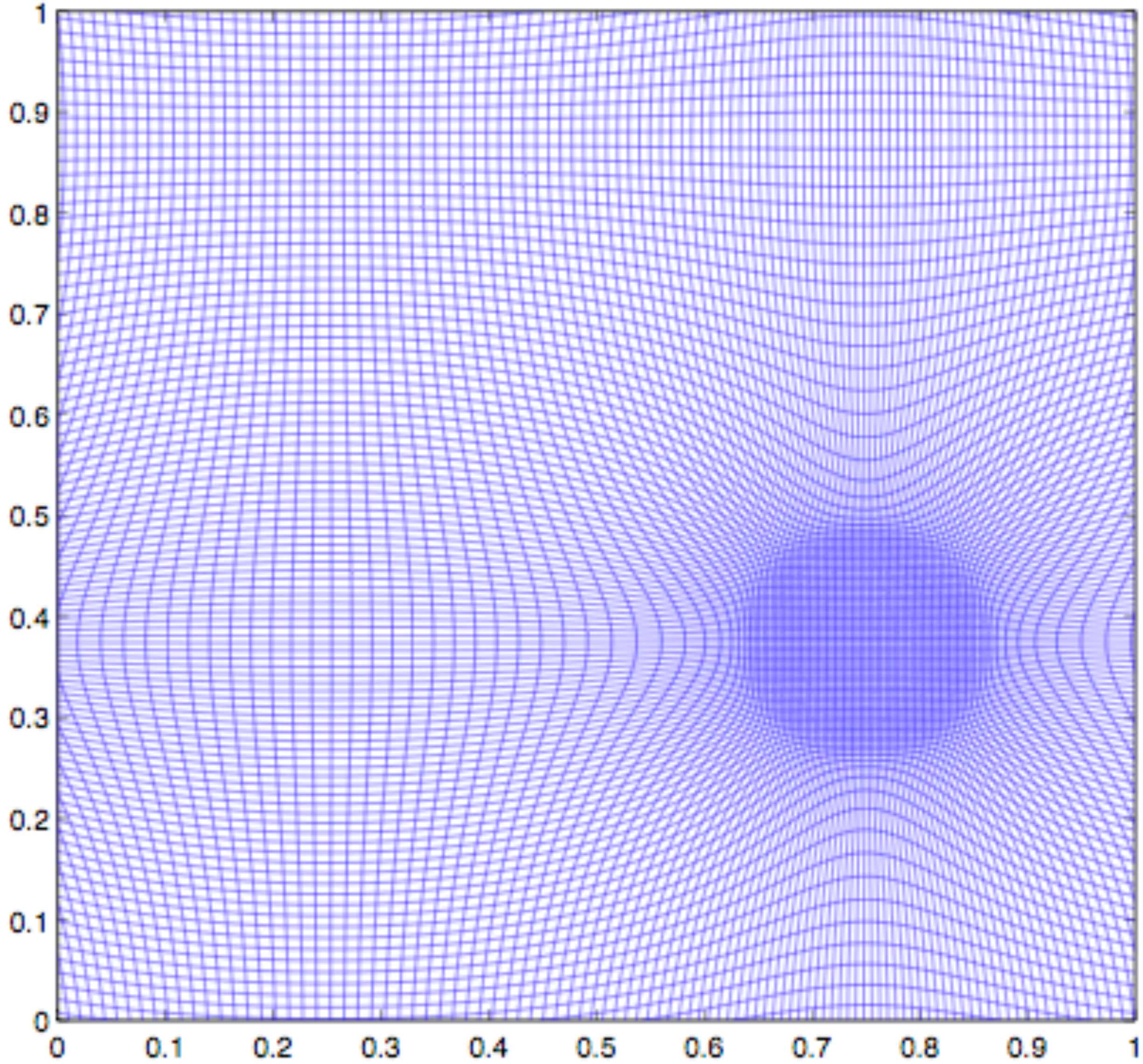
- Global and Local control of mesh regularity

eg. Good alignment properties

Traditional problems with r-adaptivity:

Mesh tangling, mesh skewness, implementation in 3D

eg. Shallow water test problem



Talk will describe an r-adaptive moving mesh method for doing this based upon geometrical ideas: optimal transport theory and Monge Ampere equations

Will demonstrate that this leads to a fast, robust and effective moving mesh method for adaptive NWP

- Which avoids mesh tangling and extreme skewness
- Works well in 1D, 2D and 3D
- Can be coupled to CFD solvers and DA codes

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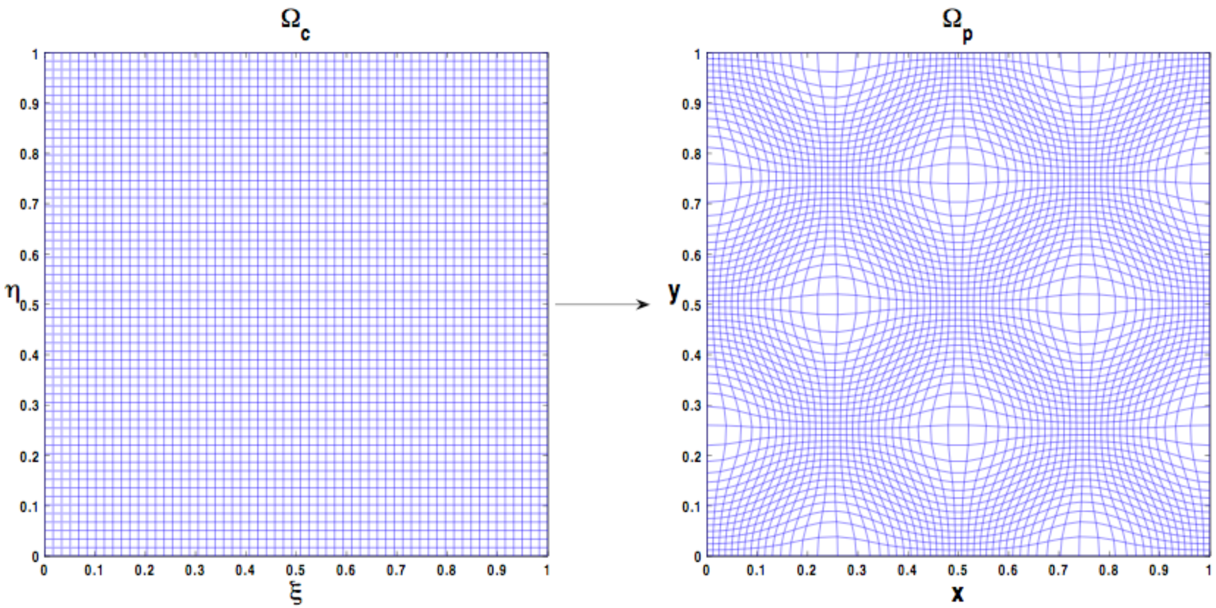
Geometrical strategy

r-adaptive methods are equivalent to MAPS

Have a computational domain $\Omega_C(\xi,\eta,\varsigma)$

Physical domain $\Omega_P(x,y,z)$

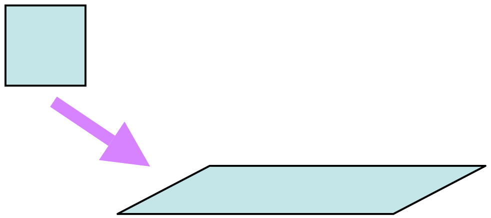
Identify a map $F(t):\Omega_C(\xi,\eta,\varsigma)\rightarrow\Omega_P(x,y,z)$



Determine F by Equidistribution

Introduce a positive unit measure $M(x,y,z,t)$ in the physical domain which controls the mesh density

A: unit set in computational domain



F(A,t) : image set

Equidistribute integral with respect to this measure

$$\int_A d\xi\, d\eta\, d\varsigma = \int_{F(A)} M(x,y,z,t)\, dx\, dy dz$$

Equidistribution minimises the maximum value of this integral

Differentiate to give:

$$M(x,y,z,t)\frac{\partial(x,y,z)}{\partial(\xi,\eta,\varsigma)} = 1$$

Basic, nonlinear, equidistribution mesh equation

Choose M to concentrate points where needed without depleting points elsewhere: error/physics/scaling

Choice of the monitor function M(X)

- Physical reasoning

eg. Potential vorticity, arc-length, curvature

- A-priori mathematical arguments

eg. Scaling, symmetry, error estimates (interpolation)

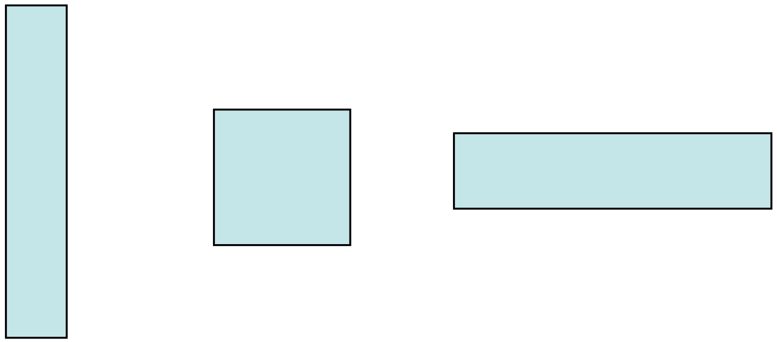
- A-posteriori error estimates (primal-dual)

eg. Residuals, super-convergence

- Data correlation estimates

Mesh construction

Problem: in two/three -dimensions equidistribution does NOT uniquely define a mesh!



All have the same area

Need additional conditions to define the mesh:

Want to avoid mesh tangling and long thin regions

Argue: A good mesh for solving a pde is often one which is as close as possible to a uniform mesh

Optimally transported meshes (Monge-Kantorovich)

Minimise

$$I(x,y,z) = \int_{\Omega_C} \left|(x,y,z) - (\xi,\eta,\varsigma)\right|^2 d\xi\, d\eta\, d\varsigma$$

Subject to

$$M(x,y,z,t)\frac{\partial(x,y,z)}{\partial(\xi,\eta,\varsigma)} = 1$$

Also used in image registration,meteorology (rearrangement of vorticity)

Optimal transport helps to prevent small angles, reduce mesh skewness and prevent mesh tangling.

Key results which makes everything work

Theorem: [Brenier]

(a) There exists a unique optimally transported mesh

(b) For such a mesh the map F is the gradient of a convex function $P(\xi,\eta,\varsigma)$

P : Scalar mesh potential $(x,y,z) = (P_\xi, P_\eta, P_\varsigma)$

$$J \equiv \frac{\partial(x,y,z)}{\partial(\xi,\eta,\varsigma)}$$ is symmetric

$\nabla \times (x,y,z) = 0$ Irrotational mesh (avoids tangling)

It follows immediately in 2D that

$$\frac{\partial(x,y)}{\partial(\xi,\eta)} = H(P) = \det\begin{pmatrix} P_{\xi\xi} & P_{\xi\eta} \\ P_{\xi\eta} & P_{\eta\eta} \end{pmatrix} = P_{\xi\xi}P_{\eta\eta} - P^2{}_{\xi\eta}$$

Hence the mesh equidistribution equation becomes

$$M(\nabla P, t)H(P) = 1 \qquad \text{(MA)}$$

Monge-Ampere equation: fully nonlinear elliptic PDE

Global and local properties of the mesh can be deduced from the regularity of the solution of the MA equation

Solve using relaxation in n Dimensions: [Russell]

$$\varepsilon\left(I-\alpha\Delta_{\xi}\right)Q_t = \left(\overline{M}(\nabla Q)H(Q)\right)^{1/n}$$

Spatial smoothing [Hou]

(Invert operator using a spectral method)

Smoothed monitor

Ensures right-hand-side scales like Q in nD to give global existence

Parabolic Monge-Ampere equation (PMA)

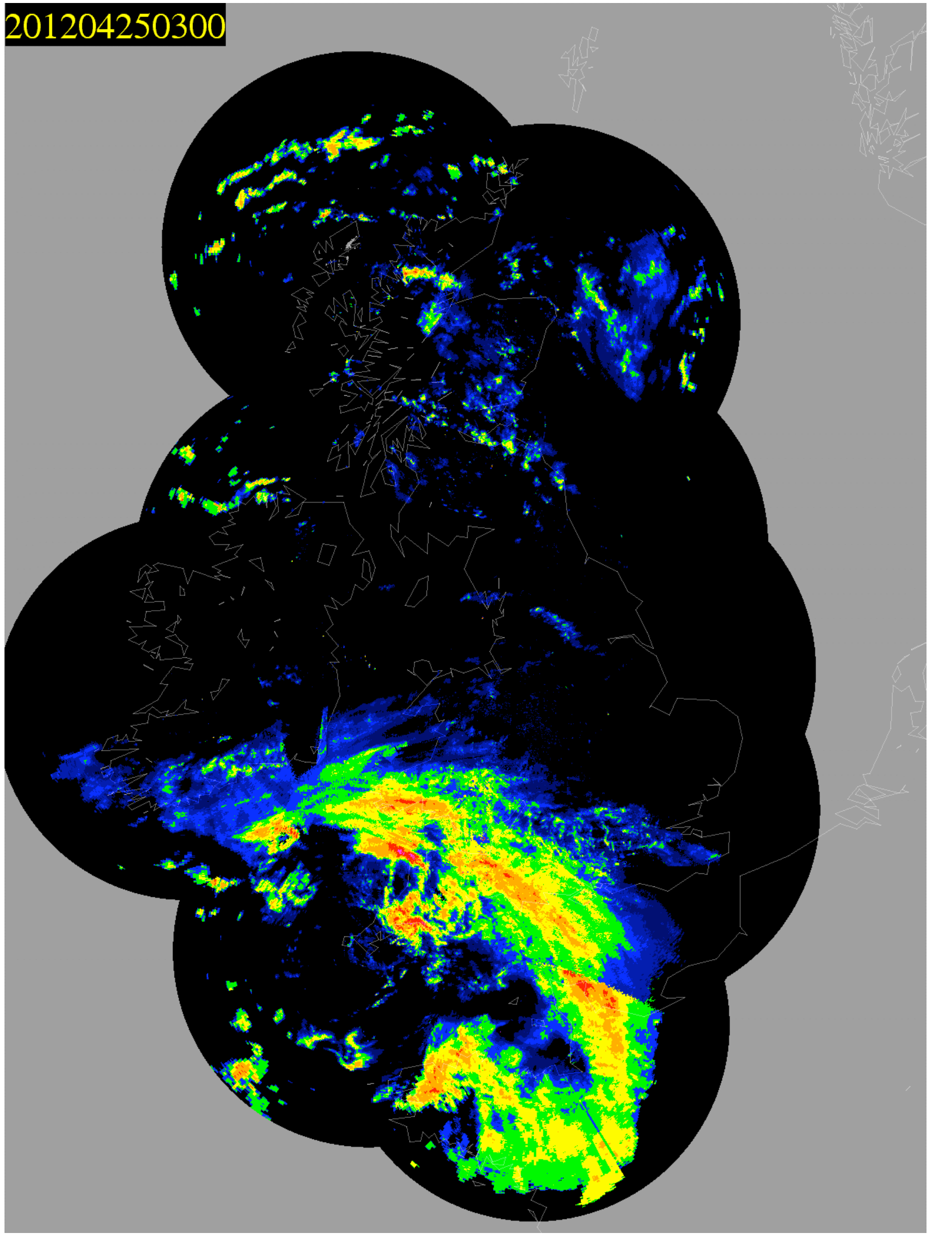
Solution Procedure

If M is prescribed then the PMA equation can be discretised in the computational domain and solved using an explicit forward Euler method.

This is a fast procedure: 5 mins for a full 3D meteorological mesh

Applications

- Image processing and image registration
- Mesh generation for meteorological Data assimilation [Browne, CJB, Cullen, Piccolo]
- Implemented in Met Office Operational Code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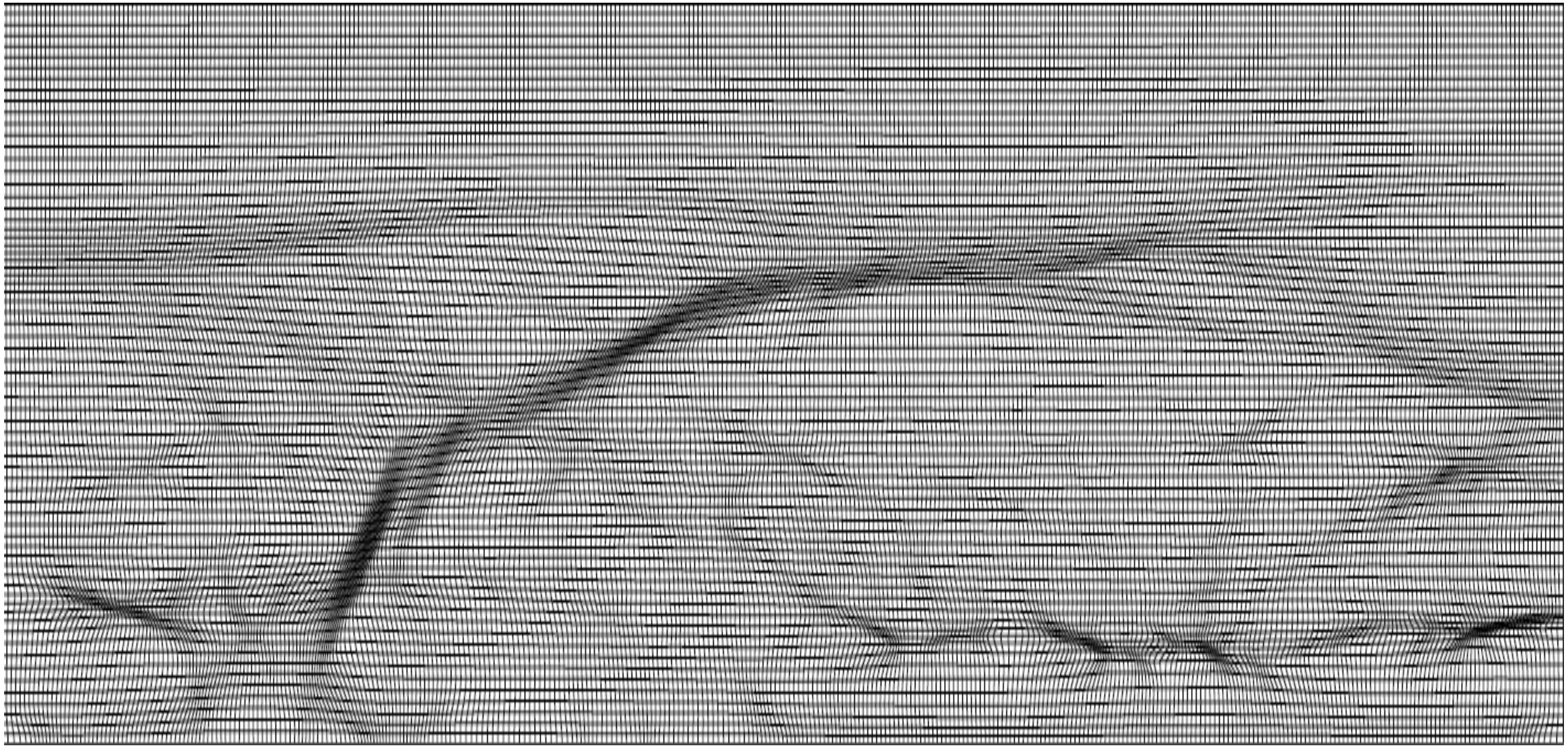
Take M to be a scaled approximation of the Potential Vorticity of the 3D flow

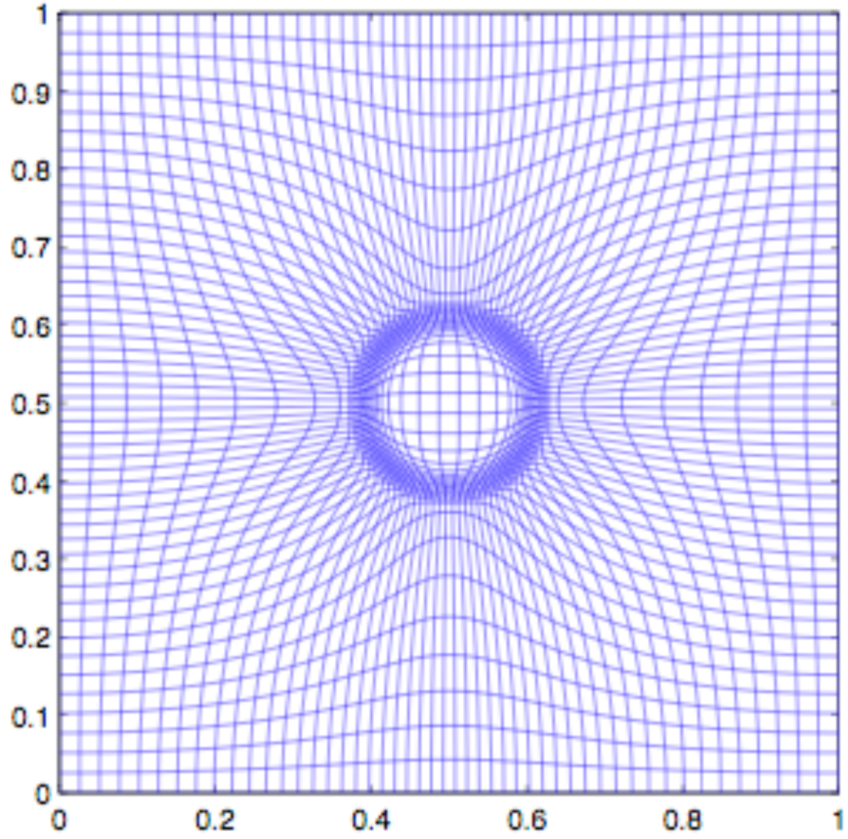


Can be coupled to DA procedure [Piccolo & Cullen]

We compute the background error covariance matrix using this adapted grid instead of the regular computational grid.

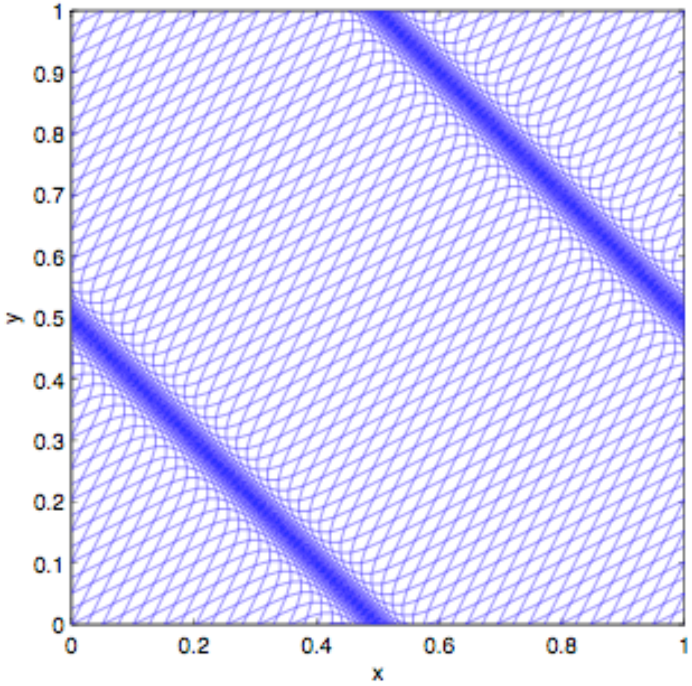
Because PMA is based on a geometric approach, it has a set of useful regularity properties

1. System invariant under translations, rotations, periodicity



Lemma 1: CJB, EJW [2012]

The solutions of the MA equation exactly align with global linear and radial features



$$J = O^T \Lambda O$$

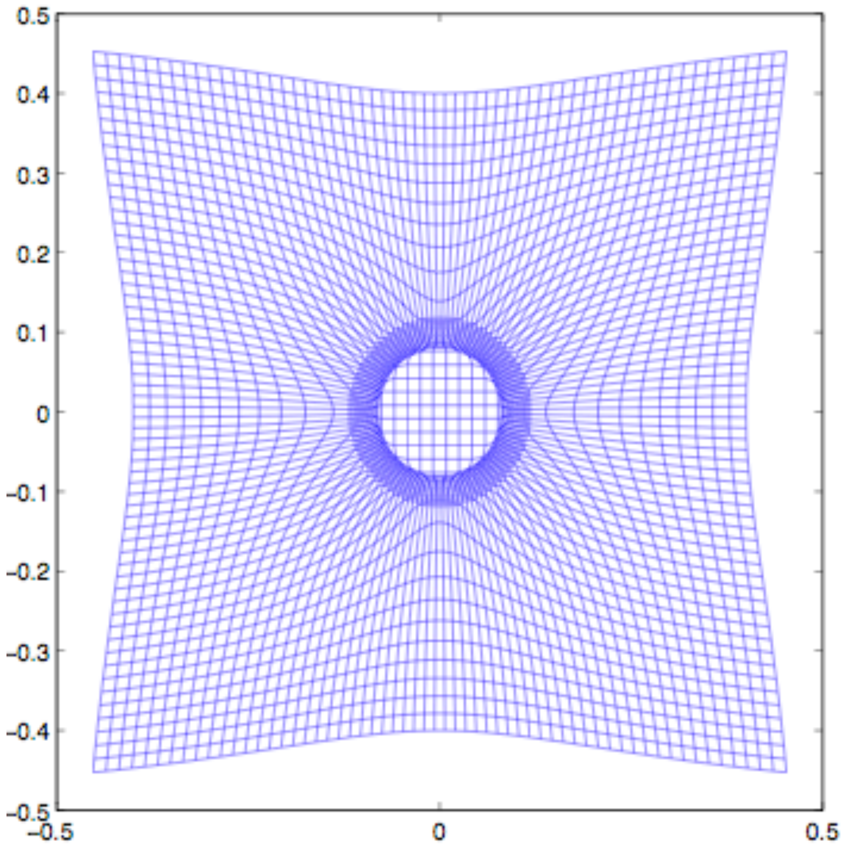
O: rotation of the linear feature

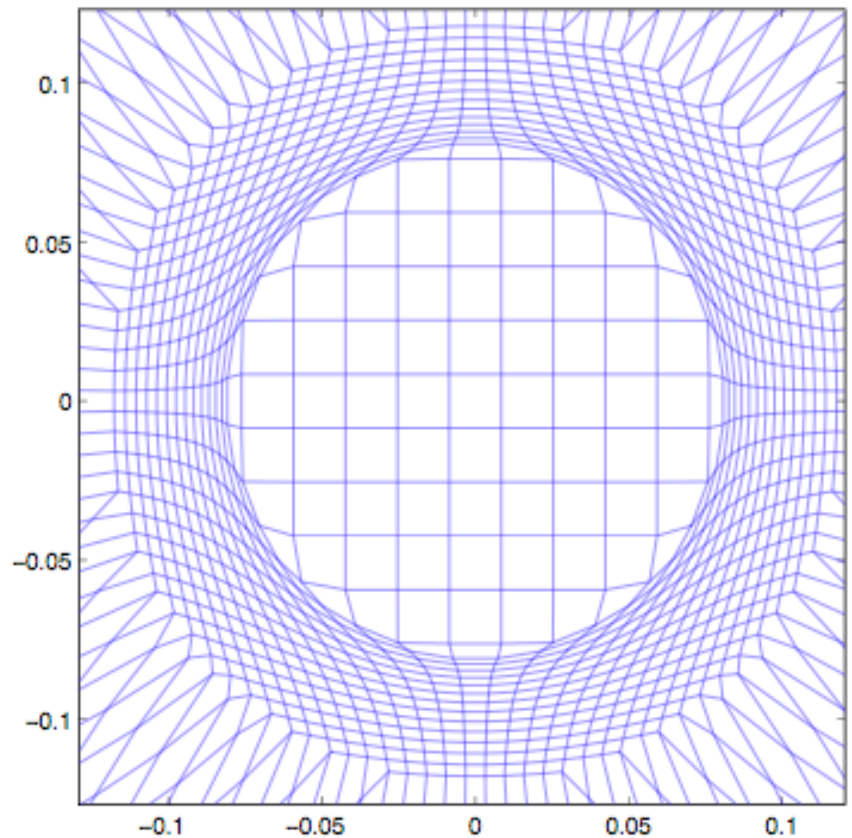
Alignment follows from a close coupling between the local structure of the solution and the global structure. This is NOT a property of other mesh generation methods

Exact solution of the MA equation

$$x = \frac{\xi R(r)}{r}, \quad y = \frac{\eta R(r)}{r}, \quad r = \sqrt{\xi^2 + \eta^2},$$

$$R(r) = \sqrt{a_i r^2 - b_i^2}, \quad i = 1,2,3$$





2. Convergence properties of PMA

Lemma 2: [Budd,Williams 2006]

(a) If M(x,t) = M(x) then PMA admits the solution

$$Q(\xi,t) = P(\xi) + \Lambda t \qquad x(\xi) = \nabla_\xi Q = \nabla_\xi P$$

(b) This solution is locally stable/convergent and the mesh evolves to an equidistributed state

Proof: Follows from the convexity of P which ensures that PMA behaves locally like the heat equation

Lemma 3: [B,W 2006]

If $M(x,t)$ is slowly varying then the grid given by PMA is epsilon close to that given by solving the Monge Ampere equation.

Lemma 4: [B,W 2006]

The mapping is 1-1 and convex for all times:

No mesh tangling or points crossing the boundary

Coupling to a PDE

In a PDE calculation M is a function of the solution of the PDE and we must couple mesh generation to the calculation of the solution

$$u_t = N(u, \nabla u, \Delta u)$$

Two methods:

1. Use the generated mesh in the physical domain and discretise the PDE in this domain using a finite element/finite volume solver.

2. Discretise PDE & PMA in the computational domain taking advantage of the simple mesh geometry

Computational Domain Scaling

$$
\begin{aligned}
u_x &= J^{-1}[y_\eta u_\xi - y_\xi u_\eta] \qquad\qquad u_y = J^{-1}[-x_\eta u_\xi + x_\xi u_\eta] \\
u_{xx} &= J{-}1[(J^{-1}y_\eta^2 u_\xi)_\xi - (J^{-1}y_\xi y_\eta u_\eta)_\xi - (J^{-1}y_\xi y_\eta u_\xi)_\eta + (J^{-1}y_\xi^2 u_\eta)_\eta] \\
u_{yy} &= J^{-1}[(J^{-1}x_\eta^2 u_\xi)_\xi - (J^{-1}x_\xi x_\eta u_\eta)_\xi - (J^{-1}x_\xi x_\eta u_\xi)_\eta + (J^{-1}x_\xi^2 u_\eta)_\eta]
\end{aligned}
$$

Jacobian J given by the mesh calculation

Other derivatives easy to find using finite difference methods

Solve the coupled mesh and PDE system either

Method One: Simultaneous Solve

Mesh and PDE as one large system (stiff!)

Lagrangian type approach.

Advantages:

No need for interpolation

Mesh and solution become one large dynamical system and can be studied as such eg. symmetries

Disadvantage: Equations are very hard to solve especially when the PDE is strongly advective (CFL condition problems)

Method 2: More suitable for PDEs with convection

By alternating between evolving the PDE and mesh

1. Time march the PDE on given mesh
2. Evolve to new mesh by solving PMA to steady state
3. Interpolate PDE solution onto the new mesh
4. Repeat from 1.

Advantages:

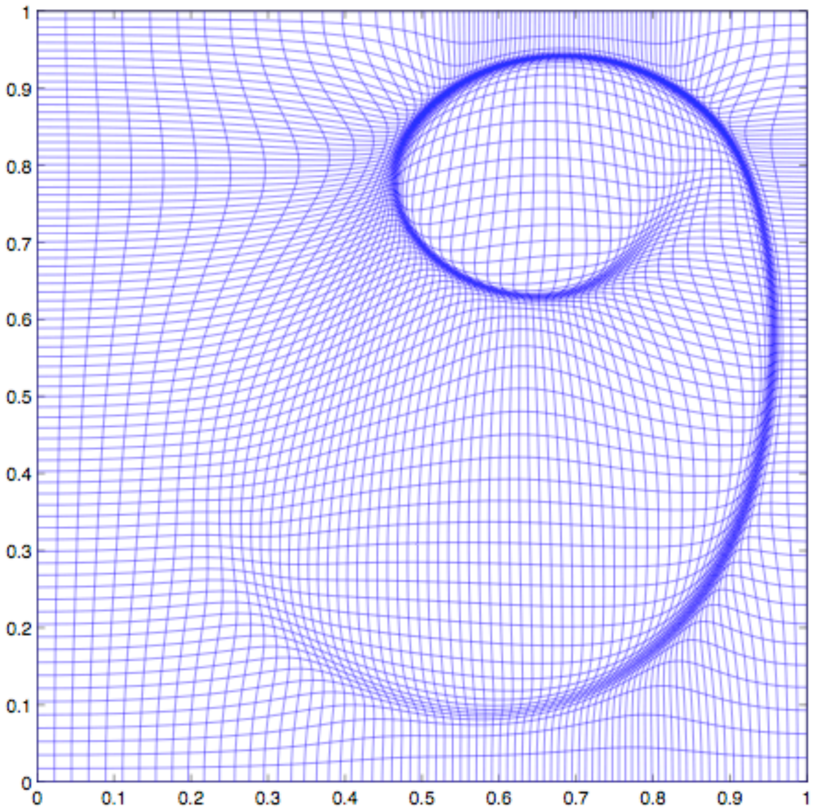
Very flexible, can build in conservation laws and incompressibility at stage 2

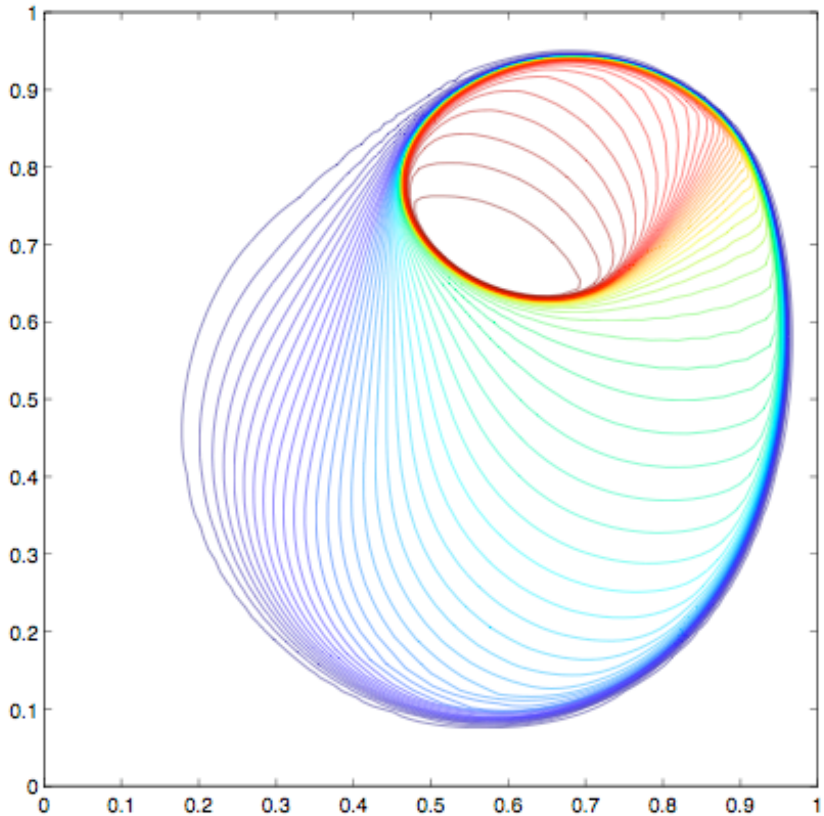
Disadvantage: Interpolation is difficult and expensive

Example 1: 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 Method 1,   M = arc-length





Example 2: Eady Problem [Cullen]

2D Eady Model

$(x, z) \in [-L, L] \times [0, H]$

$$\begin{aligned} u_t + \mathbf{u}.\nabla u - fv + \phi_x &= 0 \\ v_t + \mathbf{u}.\nabla v + fu - Cg\theta_0^{-1}(z - H/2) &= 0 \\ w_t + \mathbf{u}.\nabla w + \phi_z - g\theta\theta_0^{-1} &= 0 \\ \theta_t + \mathbf{u}.\nabla\theta - Cv &= 0 \\ \nabla.\mathbf{u} &= 0. \end{aligned}$$

$\mathbf{u} = (u, w)$ is the velocity, $\nabla = (\partial/\partial x, \partial/\partial z)$.

θ is the change in pot temp from some initial reference state θ_0.

ϕ is the pressure term.

f, g, C are constants.

Rigid lid boundary conditions: $w = 0$ at $z = 0$ and $z = H$.

All variables are periodic in x.

Initial data and parameters (Cullen, 2006).

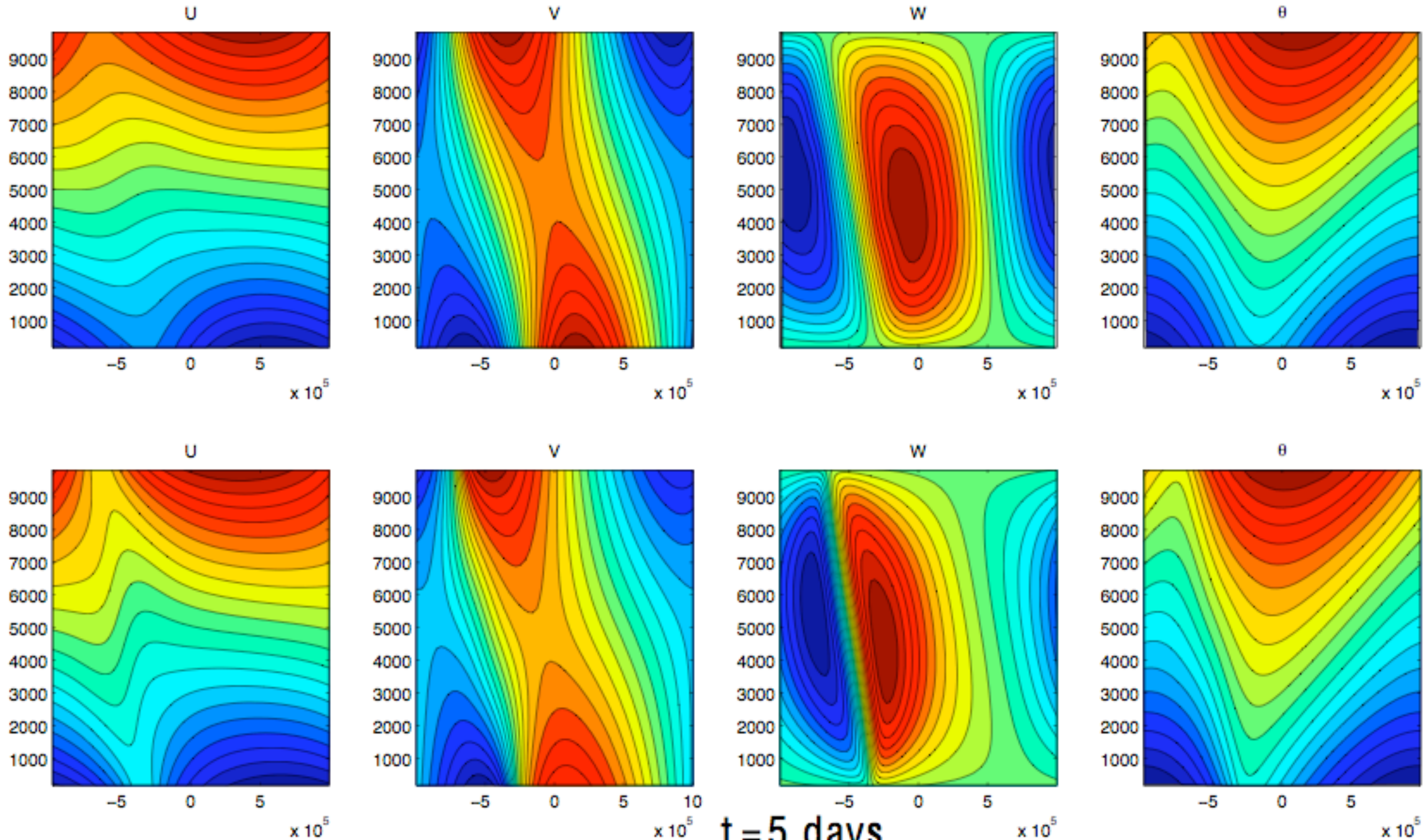
Conjectured discontinuity singularity after t = 6.3 days

M : Maximum eigenvalue R (PV = det R)

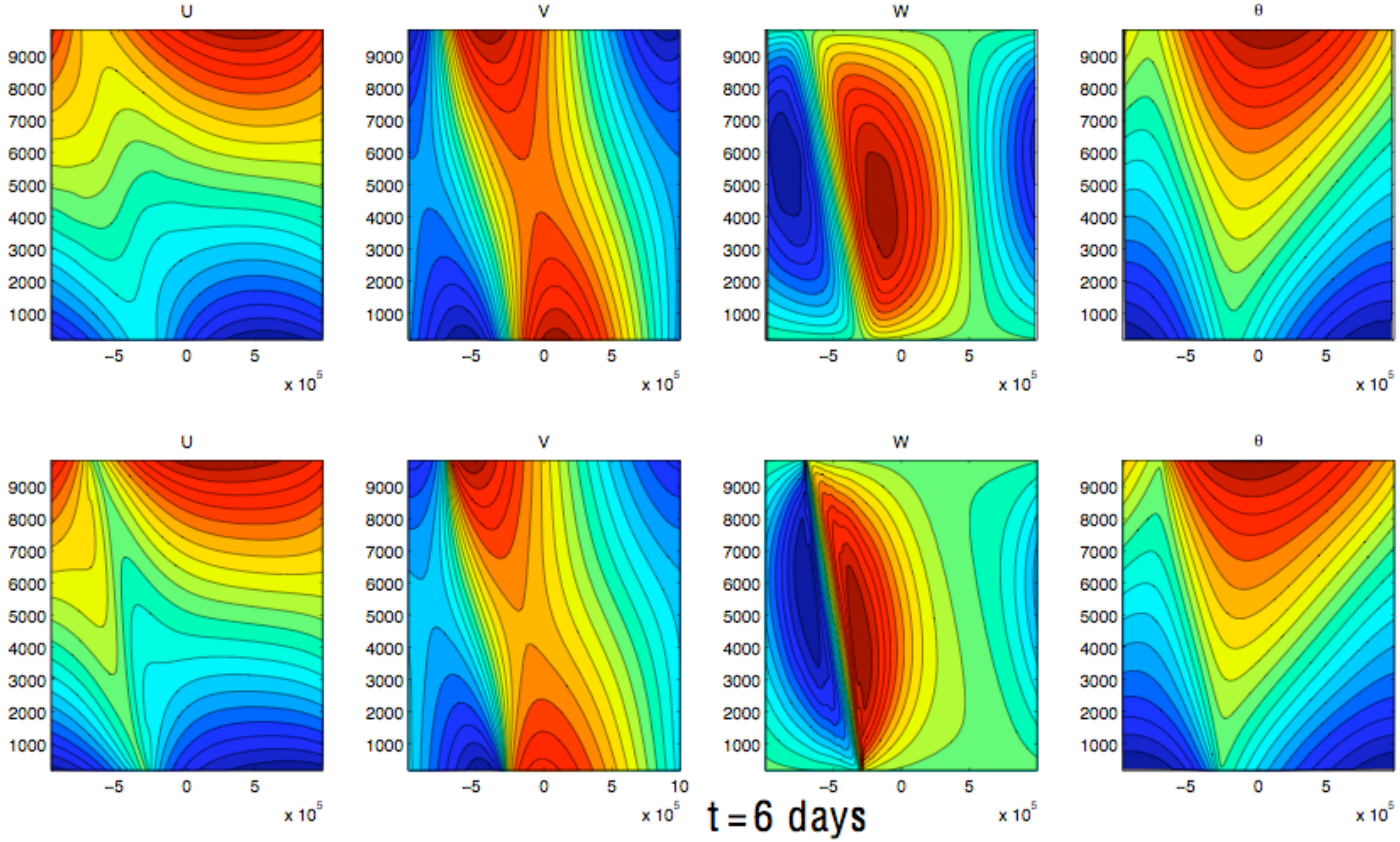
$$R = \begin{pmatrix} f^2 + f v_x & f v_z \\ g\theta_0^{-1}\theta_x & g\theta_0\theta_z \end{pmatrix}$$

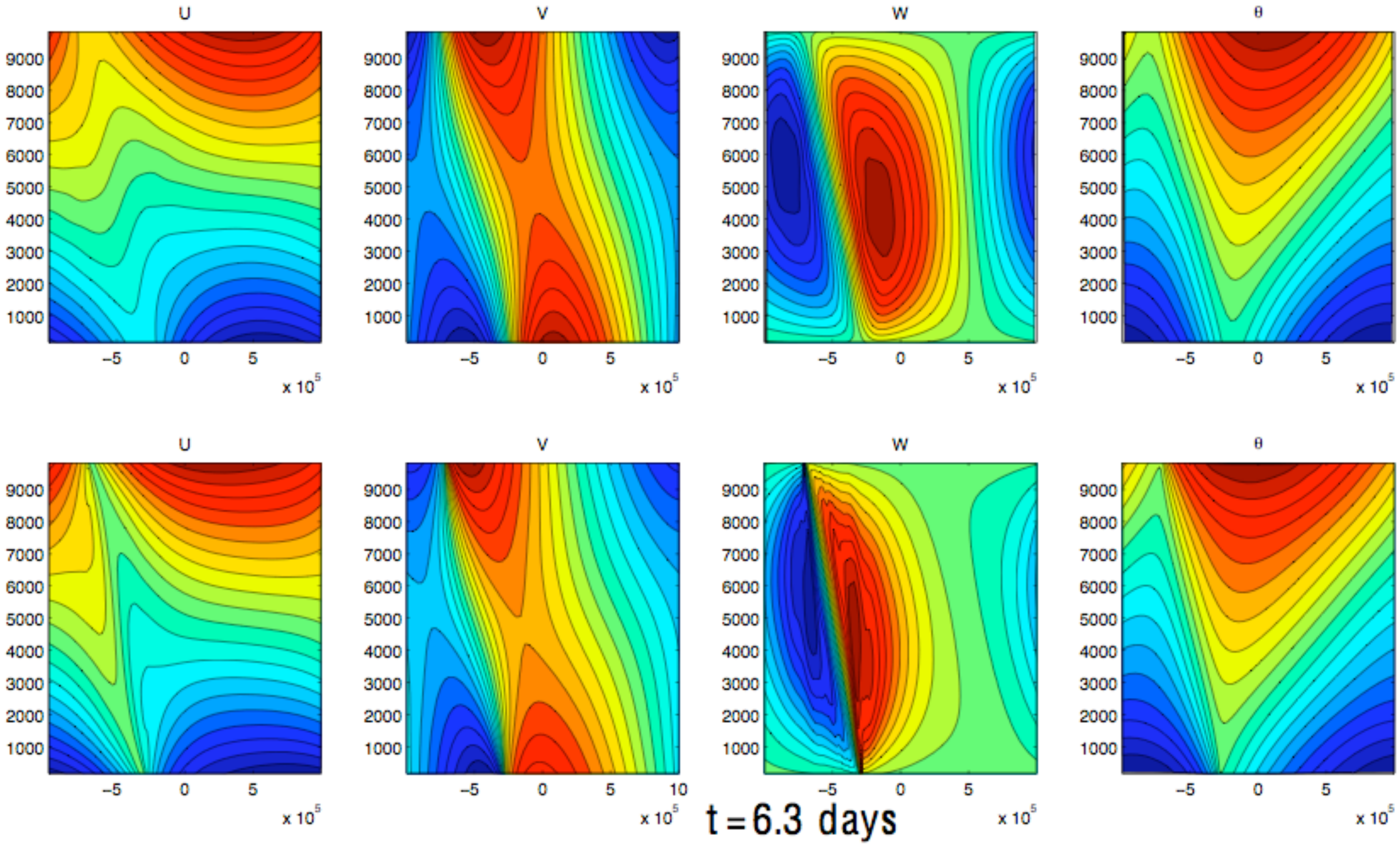
Solve using alternating Method 2:

- Finite difference method on a 60x60 Charney-Phillips mesh with pressure correction
- 2nd order interpolation [Tang] with conservation law and geostrophic balancing
- Update solution initially every 10 mins
- Update mesh every hour
- Reduce time step as singularity is approached



t = 5 days


U
V
W
θ
9000
8000
7000
6000
5000
4000
3000
2000
1000
−5
0
5
10
x 10^5
t = 6 days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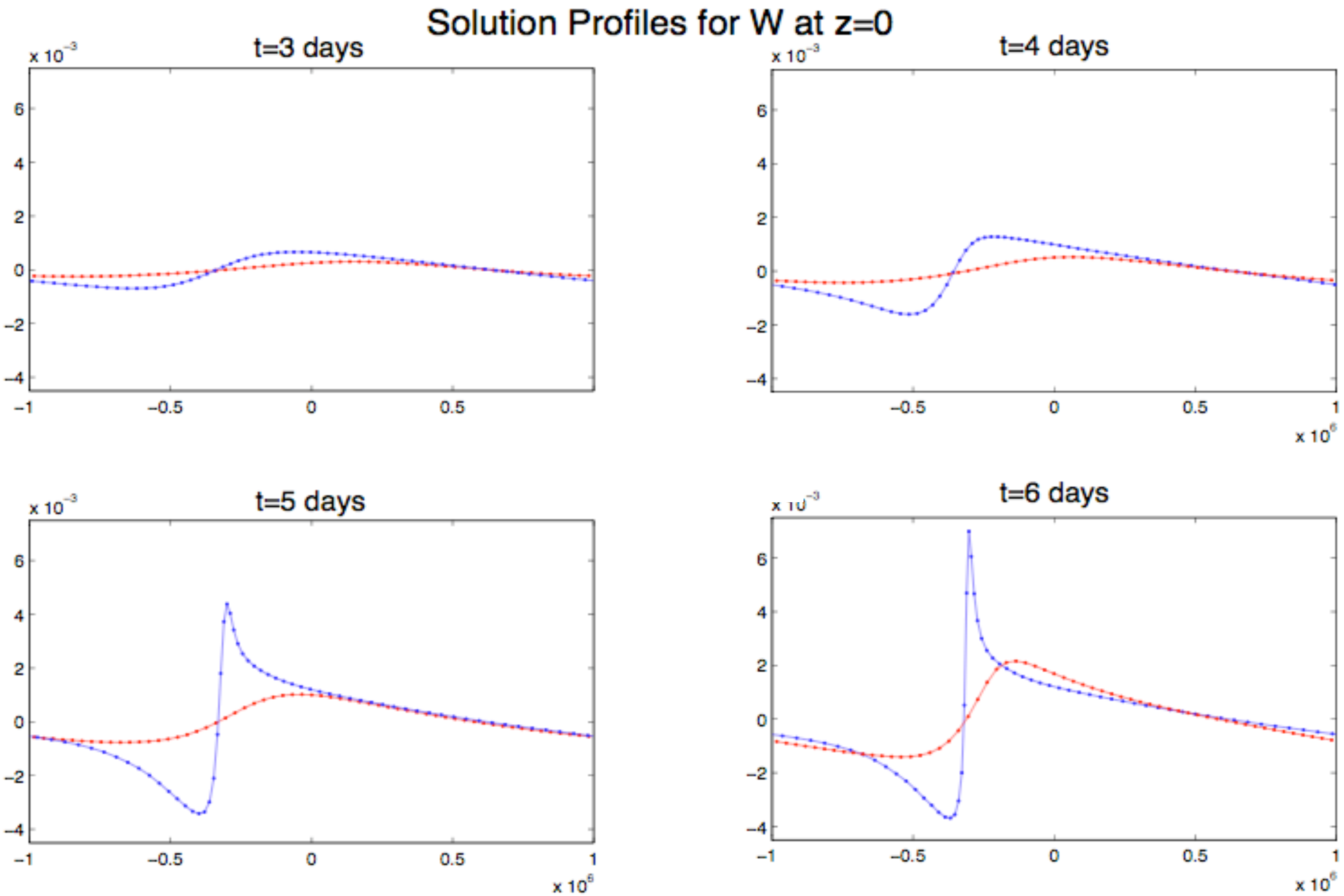
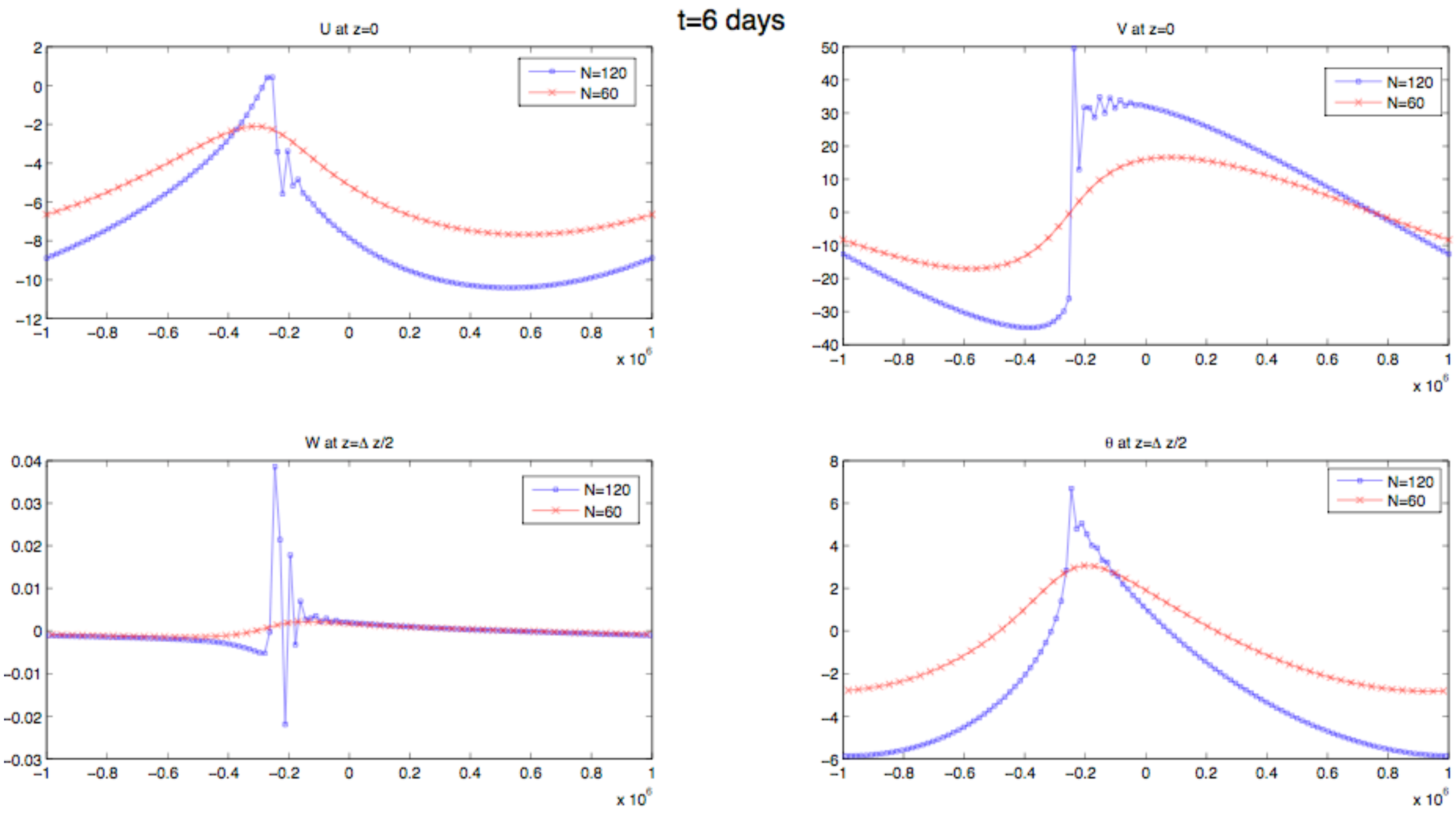
x 10^5
t = 6.3 days

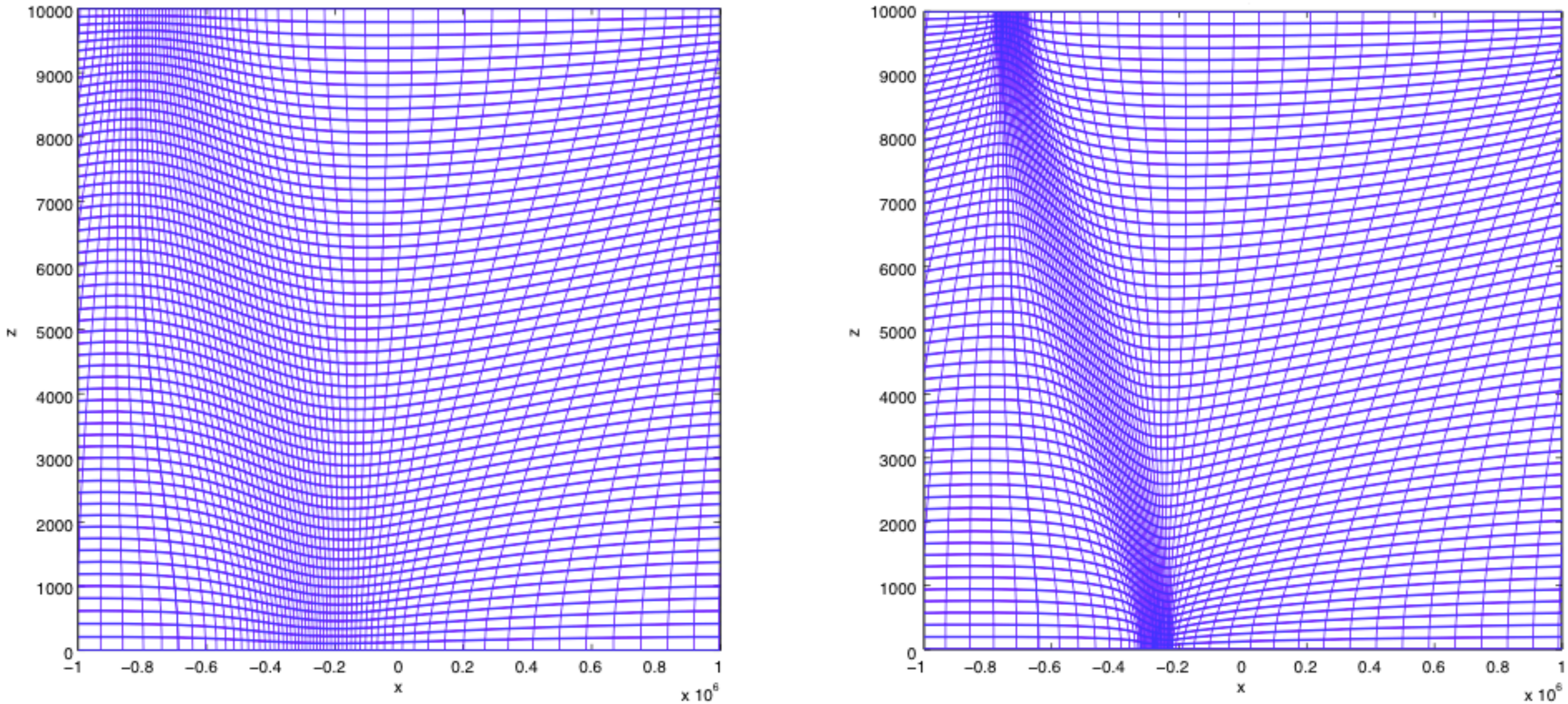
Moving mesh gives good solution profiles



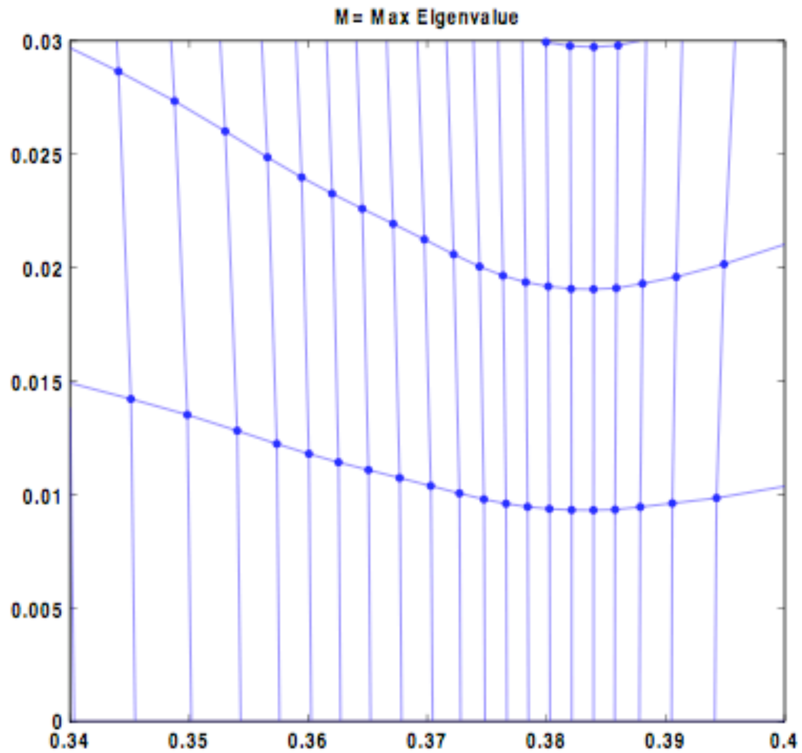
Refining uniform mesh leads to solution oscillations



Mesh profile

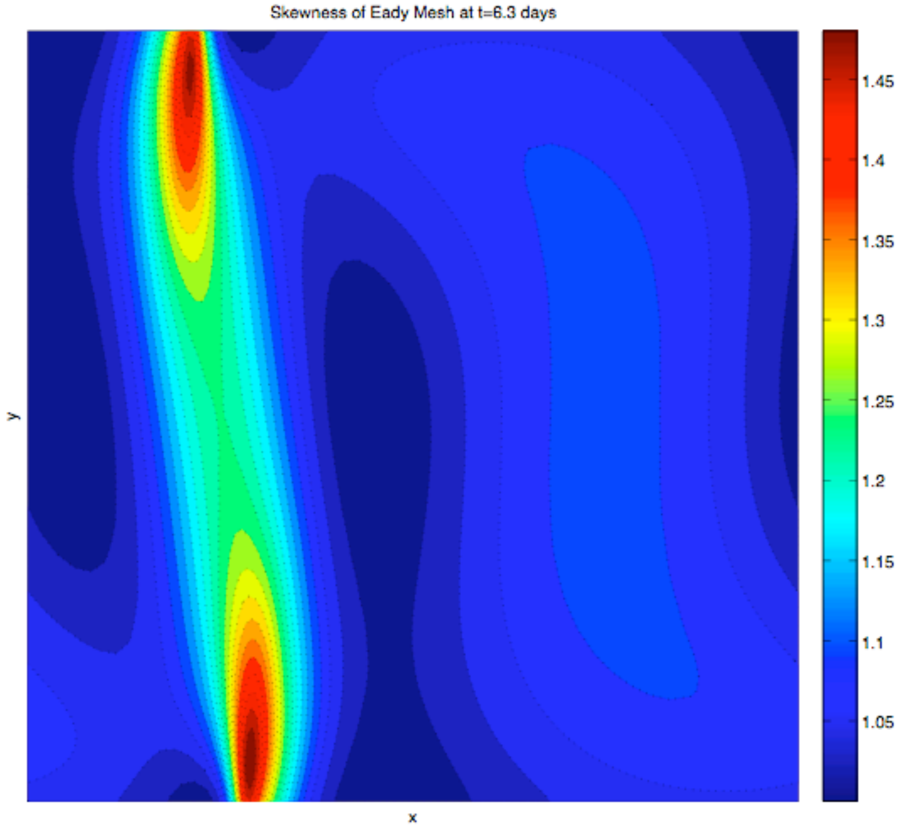


Local mesh regularity is good



Mesh Skewness is very good

$$s = \frac{\lambda_1}{\lambda_2} + \frac{\lambda_2}{\lambda_1} = \frac{tr(J^T J)}{\det(J)}$$



Conclusions

- Optimal transport is a natural way to determine moving meshes
- It can be implemented using a fast relaxation process by using the PMA algorithm
- Method works well for a variety of problems, and there are rigorous estimates about its behaviour
- Looking good on meteorological problems
- Lots of work to do to compare its effectiveness with tried and tested AMR procedures on standard test problems