Remarks on Grid Generation, Equidistribution, and Solution-adaptation

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Outline of Topics

1. Mappings, Derivatives of Mappings, Grids

2. Elliptic grid generation (PDE's)

3. Variational Methods

4. Equidistribution

5. Liao's Equidistribution Method

6. Monge-Kantorovich Approach

Part 1.

Grids, Mappings, Derivatives, Invertibility

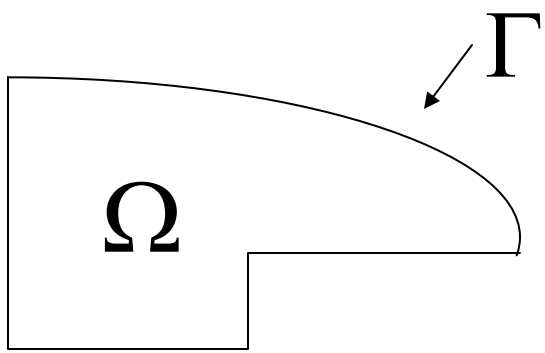
Computational Field Simulations

Numerical solution of Partial Differential Equations

<u>Typical Problem</u>: Solve the elliptic PDE

$$\nabla \bullet K \nabla u = f$$

on a domain Ω, with boundary condition $u\,|_{\Gamma} = b$



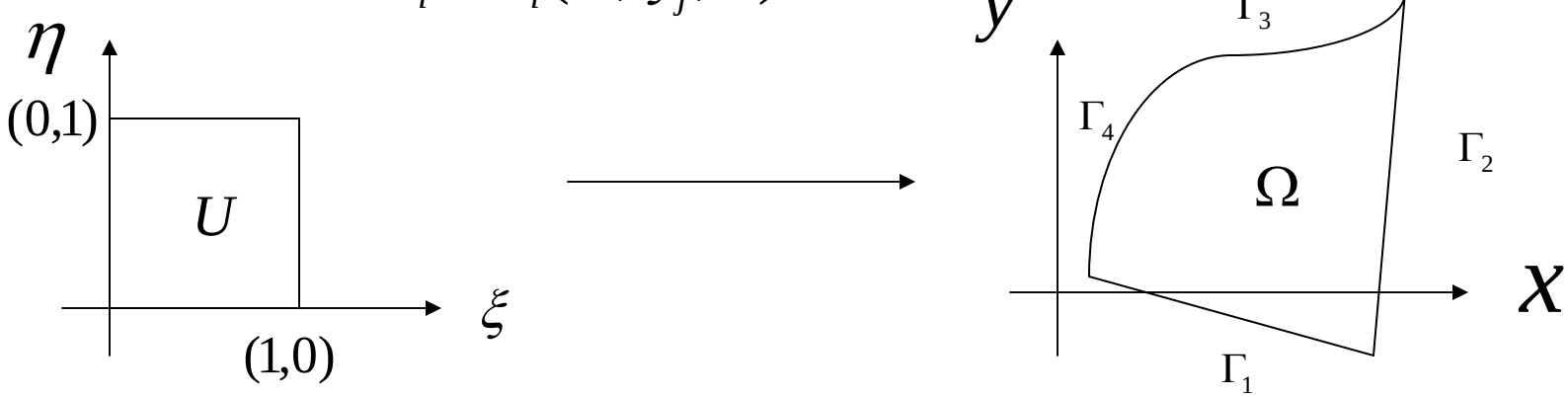
Numerical solution requires a <u>discretization</u> of the domain.

Mappings

A <u>mapping</u> is a set of functions which take points from a set U to points in a set Ω.

To solve PDE's we require the set $U \subset R^n$ to consist of the set of points $[0,1]^n$. Points in U have coordinates ξ_j which form a regular Cartesian grid (easy to discretize on this grid).

Let x_i be the coordinates of a point in Ω. Then the mapping functions are $x_i = x_i(\ldots, \xi_j, \ldots)$



The Jacobian of a Map

Assume that the map is smooth (sufficiently differentiable).

<u>Jacobian Matrix J</u>:

elements: $J_{mn} = \partial x_m / \partial \xi_n$

determinant: $\det(J) = \sqrt{g}$

The map is <u>locally invertible</u> if det(J)>0.

Example (n=2):

$$J = \begin{pmatrix} \partial x/\partial \xi & \partial x/\partial \eta \\ \partial y/\partial \xi & \partial y/\partial \eta \end{pmatrix} \qquad \det(J) = x_\xi y_\eta - x_\eta y_\xi$$

What Map Should We Use and How Do We Find It?

The map should be

- invertible,
- smooth (at least continuous & differentiable),
- have good quality (ideally, orthogonal), and
- well-adapted to the physical solution, permitting accuracy.

Coordinate Line Tangent Vectors

Columns of Jacobian Matrix are Coordinate Line Tangent Vectors

$$J = \begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix} = [\vec{x}_\xi, \vec{x}_\eta]$$

The ξ-coordinate lines of the map $\vec{x}(\xi,\eta)$ are given by holding η fixed. Thus, the tangent to a ξ-coordinate line is $\vec{x}_\xi$

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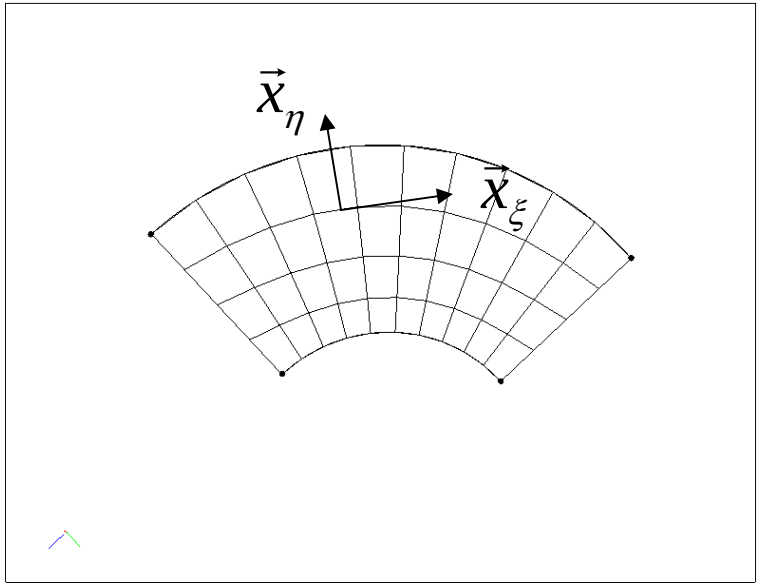


The Inverse Map & Jacobian

The inverse map $\xi(x,y);\eta(x,y)$ satisifes

$$x(\xi(x,y),\eta(x,y)) = x;\ y(\xi(x,y),\eta(x,y)) = y$$

Chain Rule:

$$x_\xi \xi_x + x_\eta \eta_x = 1;\ x_\xi \xi_y + x_\eta \eta_y = 0$$

$$y_\xi \xi_x + y_\eta \eta_x = 0;\ y_\xi \xi_y + y_\eta \eta_y = 1$$

Matrix Form:

$$\begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix}\begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Inverse Jacobian Matrix

$$J^{-1} = \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} = \left[\nabla_x \xi, \nabla_x \eta\right]^T = \tfrac{1}{\sqrt{g}}\begin{pmatrix} y_\eta & -x_\eta \\ -y_\xi & x_\xi \end{pmatrix}$$

The Metric Tensor

$$G = J^t J = \begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix}$$

$$g_{ij} = \vec{x}_{\xi_i} \cdot \vec{x}_{\xi_j}$$

$$g_{11} = \vec{x}_{\xi} \cdot \vec{x}_{\xi} = |\vec{x}_{\xi}|^2$$

$$g_{12} = \vec{x}_{\xi} \cdot \vec{x}_{\eta} = |\vec{x}_{\xi}||\vec{x}_{\eta}|\cos\vartheta$$

$$g_{22} = \vec{x}_{\eta} \cdot \vec{x}_{\eta} = |\vec{x}_{\eta}|^2$$

$$g = \det G = g_{11}g_{22} - g_{12}^2 = |\vec{x}_{\xi} \times \vec{x}_{\eta}|^2 = \left(\det(J)\right)^2$$

$$\sqrt{g} = \det(J)$$

Part 2.

Solving PDE’s to Create Grids

Elliptic Grid Generation

Elliptic Grid Generation

Winslow, 1967:

$$\nabla_x^2 \xi = 0$$

$$\nabla_x^2 \eta = 0$$

Inversion:

$$g_{22}\vec{x}_{\xi\xi} - 2g_{12}\vec{x}_{\xi\eta} + g_{11}\vec{x}_{\eta\eta} = 0$$

<u>Advantages</u>:
- mapping is smooth, C^∞
- elliptic, second-order, coupled, quasi-linear
- complete flexibility as to the boundary parameterization

<u>Disadvantages</u>:
- Relatively slow to compute the solution grids,
- Non-orthogonal, non-uniform grid lines

Invertibility Guarantee

<u>Rado's Theorem</u> (harmonic mappings): the solution map to the previous Laplace system is a one-to-one, onto provided U is convex and the boundary map is a homeomorphism. Thus *the generated grids are invertible*!

<u>Limitations</u>:

- This guarantee does not hold in three-dimensions

$$\nabla_x^2 \xi = 0$$
$$\nabla_x^2 \eta = 0$$
$$\nabla_x^2 \zeta = 0$$

- The guarantee does not hold for the Poisson System

$$\nabla_x^2 \xi = P$$
$$\nabla_x^2 \eta = Q$$

with P, Q arbitrary.

Weighted Elliptic Grid Generation

Laplace system provides no control over the interior grid

<u>Poisson System</u> (Thompson, 1974)
with P and Q 'weighting functions.'

$$\nabla_x^2 \xi = P$$
$$\nabla_x^2 \eta = Q$$

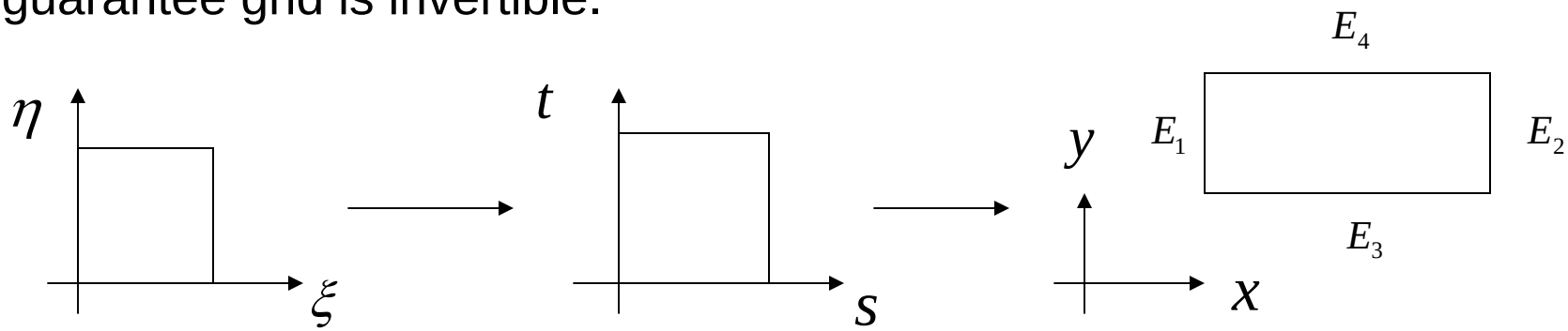
Inverted System: $g_{22}\vec{x}_{\xi\xi} - 2g_{12}\vec{x}_{\xi\eta} + g_{11}\vec{x}_{\eta\eta} = -g(P\vec{x}_{\xi} + Q\vec{x}_{\eta})$

<u>Notes</u>:
- interior grid control via P and Q (imprecise): attraction to lines or points
- widely used
- non-automatic
- no guarantee grids are smooth for arbitrary P,Q
- invertibility guarantee lost

Warsi: $$g_{22}\vec{x}_{\xi\xi} - 2g_{12}\vec{x}_{\xi\eta} + g_{11}\vec{x}_{\eta\eta} = -g_{22}P\vec{x}_{\xi} - g_{11}Q\vec{x}_{\eta}$$

Invertibility Guarantees for Weighted Elliptic Systems

Spekreijse (1995): construction of P and Q via composite mappings to guarantee grid is invertible.



Logical Space U Parameter Space P Physical Space Ω

Algebraic Map from U to P:

$$s = s_3(\xi)(1-t) + s_4(\xi)t$$

$$t = t_1(\eta)(1-s) + t_2(\eta)s$$

Elliptic Map from P to Ω:

$$s_{xx} + s_{yy} = 0$$

$$t_{xx} + t_{yy} = 0$$

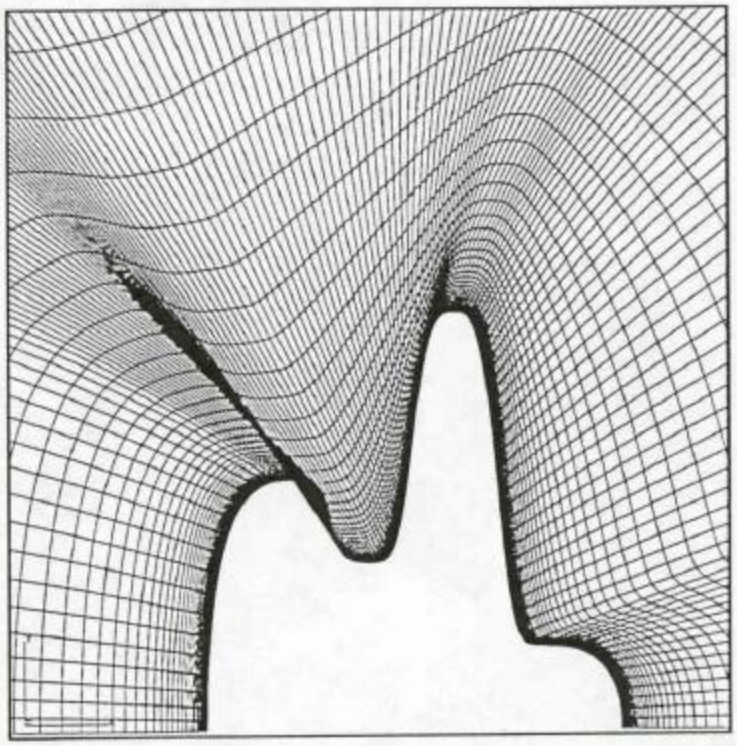


Figure 10: Initial algebraic grid with severe grid folding around a complex artificial boundary.

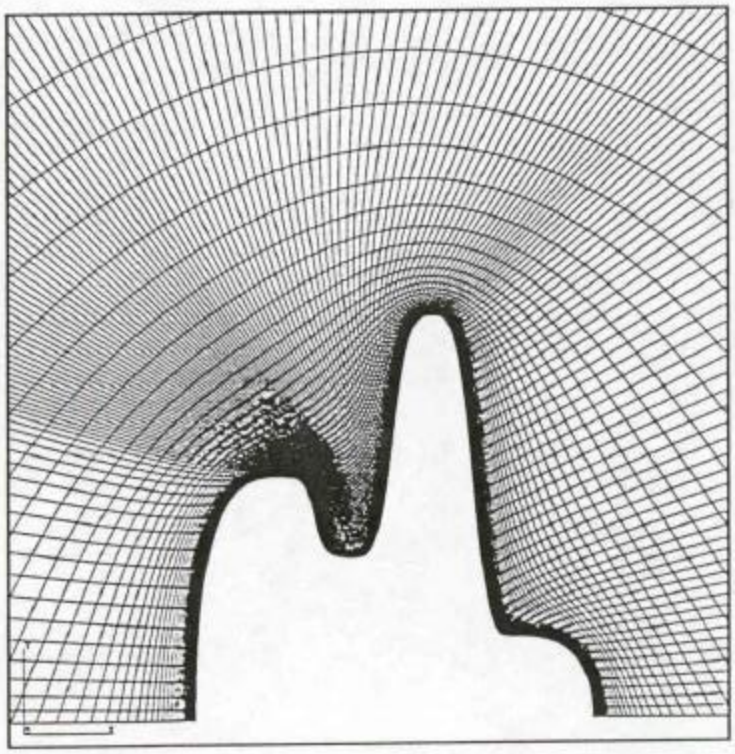


Figure 11: Elliptic grid.

Solution r-Adaptivity

Generation of grids which give the least discretization error for a fixed number of vertices.

Adapt to “solution-features” (gradients, curvature, Hessian) or to a posteriori error estimates.

Equidistribution approach to adaptivity:

- place vertices such that the local discretization error is the same everywhere in the domain.

Large error requires small cells. $|E|\Delta x = C$

Anderson area equidistribution via Poisson-like generator (inexact)

$$g_{22}\vec{x}_{\xi\xi} - 2g_{12}\vec{x}_{\xi\eta} + g_{11}\vec{x}_{\eta\eta} = \left(g_{22}\frac{w_\xi}{w} - g_{12}\frac{w_\eta}{w} \right)\vec{x}_\xi + \left(-g_{12}\frac{w_\xi}{w} + g_{11}\frac{w_\eta}{w} \right)\vec{x}_\eta$$

An exact system is derived by Kania (1999).

Part 3.

Variational Grid Generation

Variational Principle

$$I[J^{-1}] = \iint_{\Omega} F(J^{-1}) d\Omega$$

Euler-Lagrange Equations:

$$\nabla_{\xi} F - div_x \cdot \partial F / \partial J^{-1} = \vec{0}$$

Example: Brackbill-Saltzman (1982)

$$F = c_s \mid J^{-1} \mid^2 + c_a w / g \quad + c_o (\nabla_x \xi \cdot \nabla_x \eta)^2$$

Variational Grid Generation

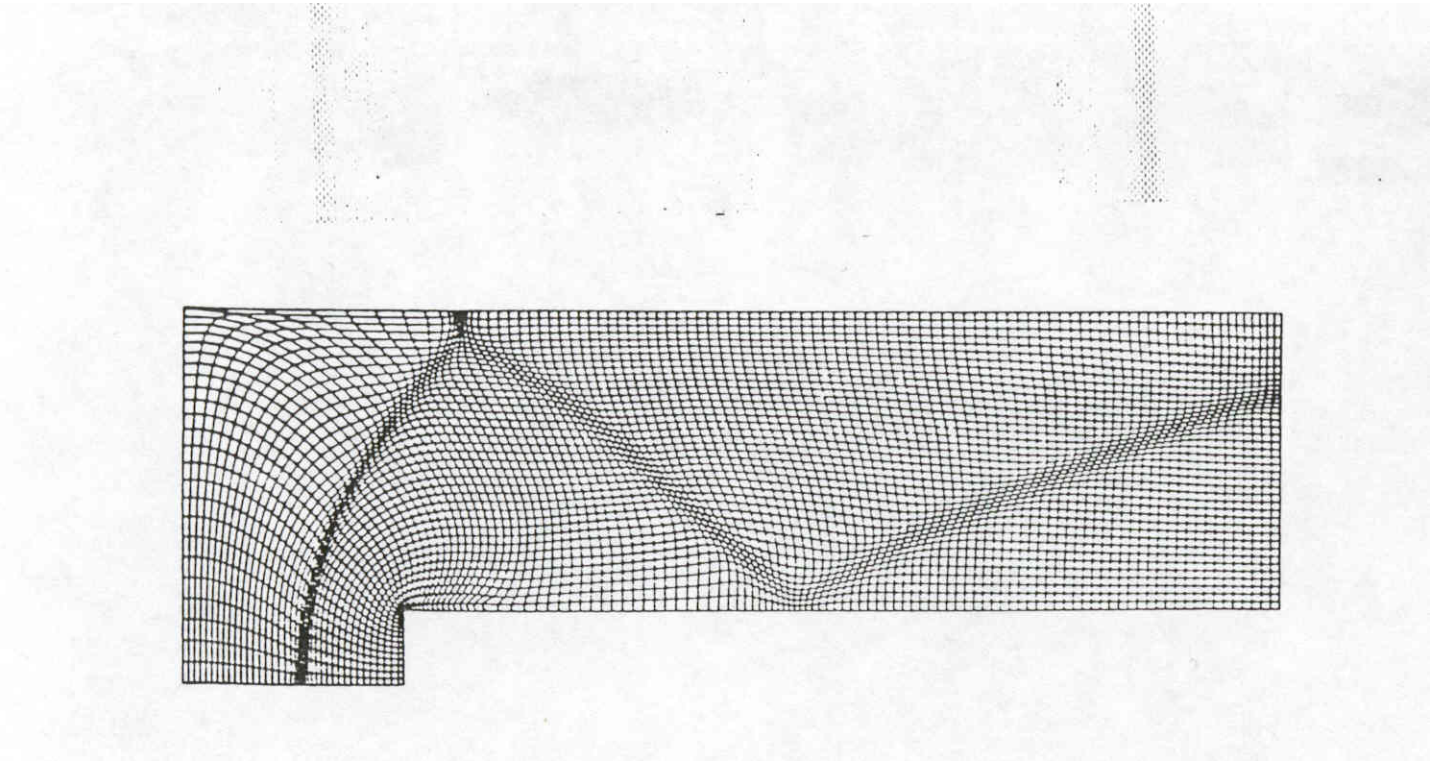
Main Attraction: If F is a grid quality metric, then that quality is (potentially) optimized. Gives less ad-hoc schemes with natural incorporation of the weights compared to PDE approach.

Notes:
- Grid is usually generated from Euler-Lagrange equations
  but can also be found by direct minimization.
- Approach not fully exploited yet.

Limitations:
- non-convex functionals, user-parameters, mixing of units
- Euler-Lagrange equations usually system of complex, non-linear PDEs
- incompatible boundary data gives ‘least-squares’ fit

Variational Mesh adapted to Shock

Brackbill-Saltzman, 1982



Harmonic Maps

Maps between manifolds $e(\xi)(u):(M,g)\rightarrow(N,h)$

Energy Density: $$e(\xi)(u)=g^{ij}(u)\frac{\partial\xi^{\alpha}(u)}{\partial u^{i}}\frac{\partial\xi^{\beta}(u)}{\partial u^{j}}h_{\alpha\beta}(\xi(u))$$

Energy Functional: $$E(\xi)=\int_{M}e(\xi)(u)dM$$

A smooth map is harmonic if it is an extremal of E

Unique Solution Guaranteed if one-to-one map between boundaries of M and N; also need boundary of manifold N convex, negative curvature.

Special Case (Winslow Variable Diffusion): $$e=\left|K\nabla\xi\right|^{2}$$

Part 4.

Equidistribution

1D Variational Example of Equidistribution

Minimize $$I[x_\xi] = \int_0^1 \frac{x_\xi^2}{2w} d\xi$$

where x is continuously differentiable and satisfies x(0)=a, x(1)=b

Usually grid is found, not by direct minimization, but by calculating the Euler-Lagrange equations (extremum is a solution to these).

One then gets the BVP $$\left(\frac{x_\xi}{w}\right)_\xi = 0$$

Integrating once, $$x_\xi = Cw(\xi)$$

Length proportional to w.

In 1D, equidistribution determines grid uniquely because the equation is linear and there is only one unknown, x.

The ratio $\frac{x_\xi}{w}$ is thus equi-distributed.

Total Error & Equidistribution

Let |E| be the Error that is to be equidistributed in 1D.

We thus want $\frac{x_\xi}{w} = |E|$

The variational principle becomes

$$I[x_\xi] = \int_0^1 \frac{x_\xi^2}{2w} d\xi = \frac{1}{2}\int_0^1 |E|\, x_\xi\, d\xi = \frac{1}{2}\int_a^b |E|\, dx$$

Thus the variational principle for equi-distribution is proportional to the Total Error.

Hence, in 1D, equi-distribution minimizes the Total Error.

2D Equidistribution

Natural generalization: $\dfrac{\sqrt{g}}{w} = C$ (local area proportional to weight)

There are two unknowns and only one equation, so grid is not uniquely determined.

Moreover, there is no rigorous connection between error equidistribution and minimization of total error. If $\dfrac{\sqrt{g}}{w} = |E|$

Then the Total Error is $\displaystyle\int_{\Omega} |E|\, dxdy = \int_0^1\int_0^1 \frac{g}{w}\, d\xi d\eta$

Minimize: $\displaystyle I\left[x_\xi, x_\eta, y_\xi, y_\eta\right] = \int_0^1\int_0^1 \frac{g}{w}\, d\xi d\eta$

Euler-Lagrange Equations are not the Equidistribution principle:

$$-\left(\frac{\sqrt{g}\, x_\eta}{w}\right)_\xi + \left(\frac{\sqrt{g}\, x_\xi}{w}\right)_\eta = 0$$

$$+\left(\frac{\sqrt{g}\, y_\eta}{w}\right)_\xi - \left(\frac{\sqrt{g}\, y_\xi}{w}\right)_\eta = 0$$

Can also do arc-length equidistribution, but this can lead to grids with bad angles and invertibility problems.

Equidistribution relation is a solution to the equations, but not the only one.

Liao's Equidistribution Method

Create C^1 mapping on Ω with <u>specified</u> <u>Jacobian</u> <u>determinant</u> (Liao, 1992).

Given a weight function *f* satisfying,

$$f(x,y) > 0 \qquad f\,|_{\partial\Omega} = 1$$

$$f \in C^1(\Omega) \qquad \iint f d\Omega = 1$$

Solve the PDE/ODE system:

$$\nabla_x \bullet \vec{v} = f - 1$$

$$D = t + (1-t)\,f$$

$$\frac{d\vec{x}}{dt} = \vec{v} / D$$

$$\vec{v} = \nabla_x \phi$$

First equation does not have unique solution.
Liao makes solution unique via a Poisson system:

$$\Delta_x \phi = f - 1$$

$$\left(\nabla_x \phi\right)|_{\partial\Omega} = 0$$

Choice is motivated by uniqueness, not by grid quality.

Proves that Jacobian of created mapping is *f*.

Monge-Kantorovich method of Equidistribution

New approach to cell-volume equidistribution based on M-K.

Minimization of grid quality measure locally constrained by the equidistribution relation. Constrained problem formulated using Lagrange multiplier, which turns out to be the solution of the M-K equation.

$$\nabla^2 \Phi + \det(H(\Phi)) = f - 1$$

Map from physical domain onto itself with

Displacement formulation: $x' = x + \nabla\Phi$

Show Jacobian of map is *f*.