Moving Adaptive Grids (part 1)

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Contents of Part 1

Grids vs. transformations:

- Different types of grids
- Benefits & possible problems
- Brief history
- Equidistribution principle

What is a(n) (adaptive) grid?

⋆ A grid (or mesh) is a discrete representation of a given domain and it is defined by specifying the position of discrete points in space as well as the interconnectivity between these points

⋆ A grid is used to represent continuous variables at fixed places and converts Partial Differential Equations (PDEs) to systems of Finite Difference, Finite Volume or Finite Element equations

⋆ An adaptive grid is a grid that reflects properties of the spatial domain and/or the PDE solution (possibly having high spatial activity in some parts of the domain)

The importance of grid generation

(Adaptive) grid generation is a necessary tool used in the numerical simulation of physical field phenomena and processes

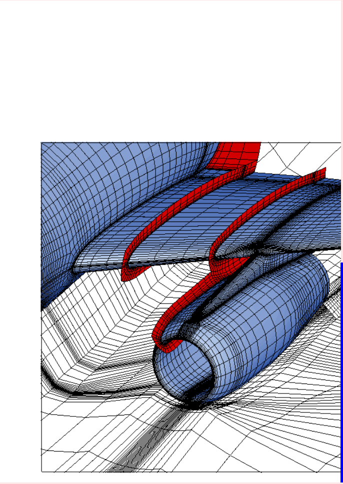
⋆ Structured grids:

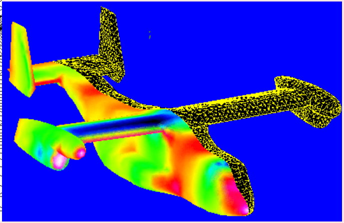
- mostly with FD's
- all elements and grid points have 'the same topology'
- 'simple' and efficient for not too complicated domains
- parallelization well-possible

⋆ Unstructured grids:

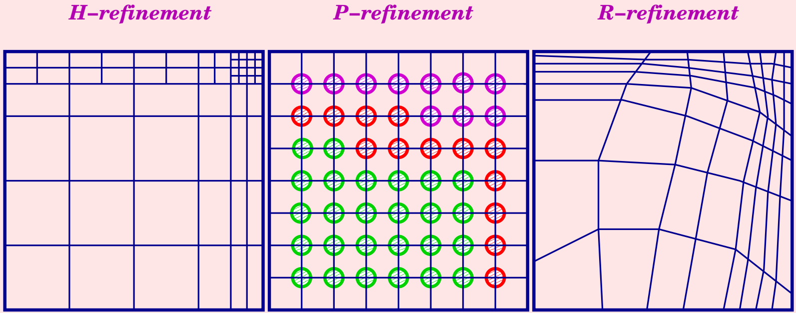
- mostly with FE's
- elements and grid points can have 'different topology'
- requires 'book-keeping' and more computer memory
- better suited for more complicated domains
- parallelization more difficult

Structured vs. unstructured grid generation





Different types of adaptive grid refinement [1]



Different types of adaptive grid refinement [2]

⋆ *h*-refinement:

- # of grid points *not* constant
- adds (or deletes) grid points
- grid equations are not coupled to physical PDEs ⇒ extra interpolation procedure needed

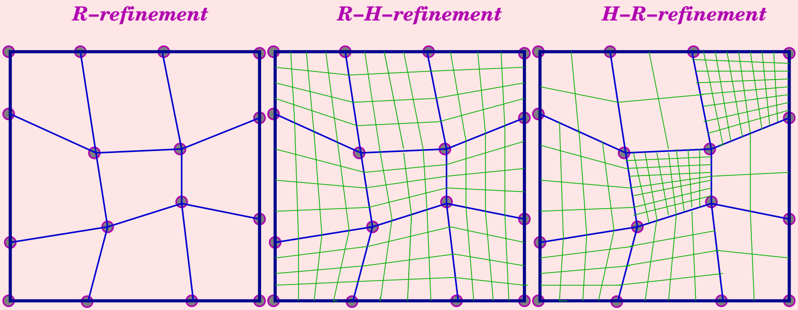
⋆ *p*-refinement:

- varies degree of piecewise polynomials (FE's)
- often in combination with *h*-refinement

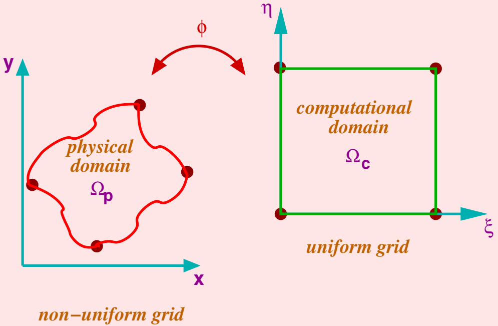
⋆ *r*-refinement:

- # of grid points *constant*
- *re*-locates (moves) grid points
- grid equations uncoupled or coupled with physical PDE

Different types of r-refinement



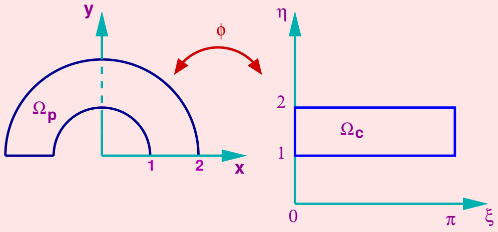
Structured r-refinement methods



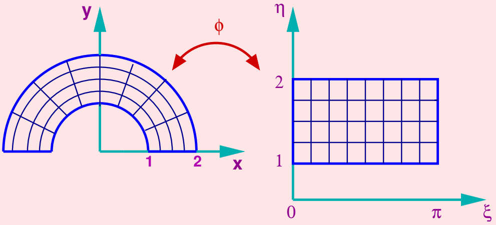
transformation $\sim$ grid

An example: polar coordinates [1]

$$\begin{cases} x(\xi,\eta) = \eta\cos(\xi) \\ y(\xi,\eta) = \eta\sin(\xi), \qquad (\xi,\eta) \in [0,\pi]\times[1,2] \end{cases}$$

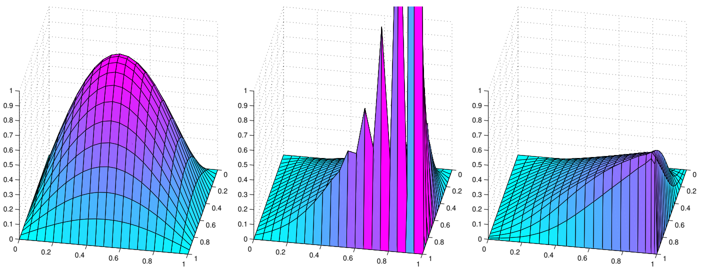


An example: polar coordinates [2]



How can adaptive moving grids help?

$$u_t = 0.005\Delta u - uu_x - uu_y$$



Initial solution, uniform grid solution & moving grid solution

What can go wrong? [1]

Consider the convection-diffusion PDE

$$\frac{\partial u}{\partial t} = \epsilon \Delta u + (x - \frac{1}{2})\frac{\partial u}{\partial x} - (y - \frac{1}{2})\frac{\partial u}{\partial y} + f(x, y, t)$$

where

$$f(x, y, t) = u_t^* - \epsilon \Delta u^* - (x - \frac{1}{2})\frac{\partial u^*}{\partial x} + (y - \frac{1}{2})\frac{\partial u^*}{\partial y}$$

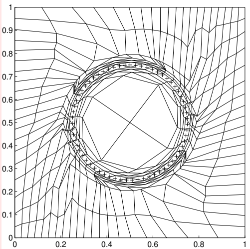
such that

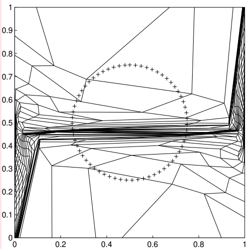
$$u^*(x, y, t) = \tfrac{1}{2}(1 - e^{-t})(1 + \tanh(100(\tfrac{1}{16} - (x - \tfrac{1}{2})^2 - (y - \tfrac{1}{2})^2)))$$

is the exact solution of the PDE model *independent of* ϵ

What can go wrong? [2]

For 'some method', we may get for $\epsilon = \mathcal{O}(1)$ (left) & $0 < \epsilon \ll 1$



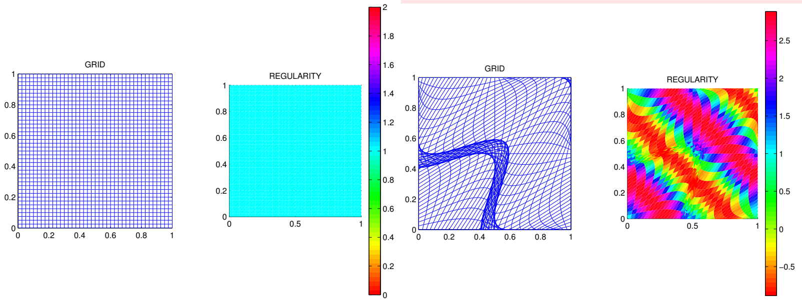


What can go wrong? [3]

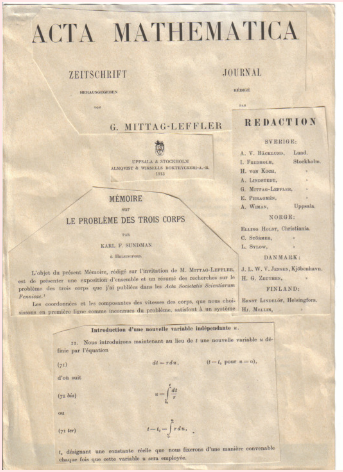
For ‘another‘ method, we may have

$$\begin{aligned} x(\xi,\eta,\theta) = &\quad \xi + \epsilon\ \theta \sin(2\pi\xi)\sin(2\pi\eta), \epsilon = 0.1 \\ y(\xi,\eta,\theta) = &\quad \eta + \epsilon\ \theta \sin(2\pi\xi)\sin(2\pi\eta), t = \theta \end{aligned}$$

(non-singularity of the mapping $\sim \mathcal{J} := x_\xi y_\eta - x_\eta y_\xi > 0$)



Historical overview [1]



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MÉMOIRE sur LE PROBLÈME DES TROIS CORPS

PAR KARL F. SUNDMAN à Helsingfors.

L'objet du présent Mémoire, rédigé sur l'invitation de M. Mittag-Leffler, est de présenter une exposition d'ensemble et un résumé des recherches sur le problème des trois corps que j'ai publiées dans les *Acta Societatis Scientiarum Fennicae*.[1]

Les coordonnées et les composantes des vitesses des corps, que nous choisissons en première ligne comme inconnues du problème, satisfont à un système

Introduction d'une nouvelle variable indépendante u.

11. Nous introduirons maintenant au lieu de t une nouvelle variable u définie par l'équation

(71) $$dt = r\,du, \qquad (t = t_0 \text{ pour } u = 0),$$

d'où suit

(71 *bis*) $$u = \int_{t_0}^{t} \frac{dt}{r}$$

ou

(71 *ter*) $$t - t_0 = \int_0^u r\,du,$$

t_0 désignant une constante réelle que nous fixerons d'une manière convenable chaque fois que cette variable u sera employée.

Historical overview [2]

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A COORDINATE SYSTEM HAVING SOME SPECIAL ADVANTAGES FOR NUMERICAL FORECASTING

By N. A. Phillips

Massachusetts Institute of Technology[1]

(Manuscript received 29 October 1956)

The coordinate system used to date in numerical forecasting schemes has been the x, y, p, t-system introduced by Sutcliffe and Godart [4] and also by Eliassen [3]. This system, in common with the ordinary x, y, z, t-system, has certain computational disadvantages in the vicinity of mountains, because the lower limit of the atmosphere is not a coordinate surface. The purpose of this brief note is to describe a modified coordinate system in which the ground is always a coordinate surface.

It is obtained by replacing the vertical coordinate p in the x, y, p, t-system by the independent variable $\sigma = p/\pi$, where $\pi = \pi(x, y, t)$ is the pressure at ground level. σ ranges monotonically from zero at the top of the atmosphere to unity at the ground. In describing the relation between this x, y, σ, t-system and the usual x, y, p, t-system, we will use a subscript p to indicate a derivative along a pressure surface. Differentiation in the new x, y, σ, t-system will have no subscripts.

The following relation holds, where ξ can be x, y, or t:

$$\left(\frac{\partial}{\partial \xi}\right)_p = \frac{\partial}{\partial \xi} - \frac{\sigma}{\pi}\frac{\partial \pi}{\partial \xi}\frac{\partial}{\partial \sigma}.$$

The horizontal equations of motion then become

$$\frac{du}{dt} = fv - \frac{\partial \phi}{\partial x} + \frac{\sigma}{\pi}\frac{\partial \phi}{\partial \sigma}\frac{\partial \pi}{\partial x} + F_x, \qquad (1)$$

and

$$\frac{dv}{dt} = -fu - \frac{\partial \phi}{\partial y} + \frac{\sigma}{\pi}\frac{\partial \phi}{\partial \sigma}\frac{\partial \pi}{\partial y} + F_y, \qquad (2)$$

where F_x and F_y are the horizontal components of the frictional force per unit mass, $u = dx/dt$, $v = dy/dt$, f is the Coriolis parameter, and ϕ is the geopotential. As is customary in most meteorological work, the Coriolis terms proportional to the cosine of the latitude have been neglected. Equations (1) and (2) differ from those in the x, y, p, t-system only by the inclusion of the terms in $\partial\phi/\partial\sigma$.

The operator d/dt is given by

$$\frac{d}{dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + \dot{\sigma}\frac{\partial}{\partial \sigma}, \qquad (3)$$

where $\dot{\sigma} = d\sigma/dt$.

The hydrostatic equation is obtained from the relation

$$\frac{\partial}{\partial p} = \frac{\partial \sigma}{\partial p}\frac{\partial}{\partial \sigma} = \frac{1}{\pi}\frac{\partial}{\partial \sigma},$$

and becomes, simply,

$$\partial\phi/\partial\sigma = -RT/\sigma. \qquad (4)$$

Here R is the gas constant, and T is the absolute temperature. The coefficient $\pi^{-1}\sigma(\partial\phi/\partial\sigma)$ appearing in (1) and (2) can thus be replaced by $-RT/\pi$. Since ϕ is known at $\sigma = 1$ (at the ground), a knowledge of $T(\sigma)$ will give $\phi(\sigma)$ from (4) by integration.

The equation of continuity in the x, y, p, t-system is

$$\nabla_p \cdot \mathbf{v} + \partial\omega/\partial p = 0,$$

where $\omega = dp/dt$, and $\mathbf{v}$ is the horizontal velocity. Introducing the relation $dp/dt = \pi\dot{\sigma} + \sigma(d\pi/dt)$, we obtain the continuity equation in the new system:

$$\nabla \cdot \pi\mathbf{v} + \pi\,\partial\dot{\sigma}/\partial\sigma + \partial\pi/\partial t = 0. \qquad (5)$$

Since $\dot{\sigma}$ is zero at the top of the atmosphere ($\sigma = 0$), integration of (5) with respect to σ gives

$$\pi\dot{\sigma} = -\int_0^{\sigma} \nabla \cdot \pi\mathbf{v}\, d\sigma - \sigma\frac{\partial \pi}{\partial t}. \qquad (6)$$

Extension of the integration all the way to the ground ($\sigma = 1$) gives the formula for $\partial\pi/\partial t$:

$$\frac{\partial \pi}{\partial t} = -\int_0^1 \nabla \cdot \pi\mathbf{v}\, d\sigma, \qquad (7)$$

since $\dot{\sigma} = 0$ at the ground.

[1] The research reported here has been sponsored by the Geophysics Research Directorate, Air Force Cambridge Research Center, and by the Office of Naval Research under Contract Nonr-1841(18).

Historical overview [3]

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- Survey paper by Thompson, 1985, 'Dynamically-adaptive grids'
- Survey paper by Eiseman, 1987, 'Adaptive grid generation'
- Survey paper by Hawken et al, 1991, 'Adaptive node-movement techniques'
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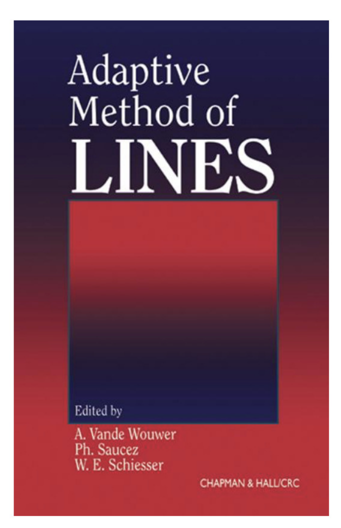
Historical overview [4]

- papers by Russell, Huang, Cao, ... (Vancouver, Kansas)
- papers by Miller, Baines, Carlson, Jimack, ... (Berkeley, Reading)
- papers by Liao, Liu, Anderson, ... (Arlington, Texas)
- papers by Blom, Verwer, Zegeling, ... (Amsterdam, Utrecht)
- papers by Ivanova, Degtyarev, ... (Keldysh institute, Moscow)
- papers by Tao Tang and co-authors (Hong Kong, Beijing)
- papers by Mackenzie, Sloan, Beckett, ... (Strathclyde)
- papers by Williams, Stockie, Budd, ... (Vancouver, Bath)
- many others...!

Literature [1]



CRC Press

Literature [2]

Weizhang Huang • Robert D. Russell

Adaptive Moving Mesh Methods

Springer

Book, 2011

Literature [3]

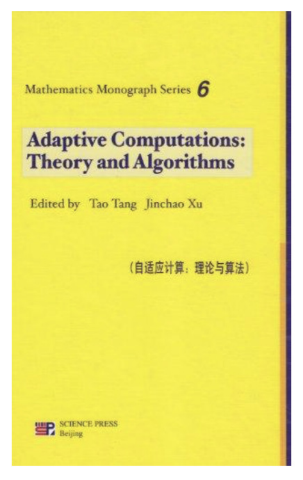
Go with the Flow

Moving meshes and solution monitoring for compressible flow simulation

Arthur van Dam

Utrecht, 2009

Literature [4]



Beijing, 2007

Literature [5]

Budd, C., Huang, W., & Russell, R. (2009). Adaptivity with moving grids. *Acta Numerica, 18*, 111-241.

Acta Numerica, 2009

Transformation vs. grid [1]

non-uniform grid in x-direction $\sim$ uniform grid in ξ-direction

transformation nonsingular $\Leftrightarrow$ Jacobian $\neq 0$

$\sim$ grid remains undistorted

$\sim$ computations do not break down

Transformation vs. grid [2]

Example 1:

$x(\xi) = \xi^2$, with $\xi \in [0,1]$ and $x \in [0,1]$ has Jacobian
$\mathcal{J} = \frac{dx}{d\xi} = 2\xi > 0$ for $\xi > 0$.

Example 2:

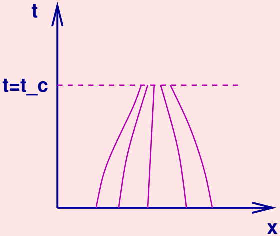
constants $A,\ B,\ C,\ D$ can be found with
$x(\xi) = A + B\xi + C\xi^2 + D\xi^3$ and $x(0) = 0, x(1) = 1, x(\frac{1}{2}) = \frac{1}{2}$ but also $\frac{dx}{d\xi}(\frac{1}{2}) = 0$. This gives a singular transformation (grid crossing in the non-uniform grid).

Transformation vs. grid [3]

Example 3:

consider the PDE $u_t = -\beta(u)u_x + \gamma(u)$. The 'Method of Characteristics' (MoC) defines (implicitly) a transformation $(x(\xi,\theta), t = \theta)$, $\Rightarrow$ grid, that must satisfy $\frac{\partial x}{\partial \theta} = \beta(u)$, $\frac{\partial u}{\partial \theta} = \gamma(u)$.

A special case with $\beta(u) = u$, $\gamma(u) = 0$, inviscid Burgers' equation, gives $\frac{\partial x}{\partial \xi} = 0$ at $t = t_{crit}$ (transformation becomes singular $\sim$ characteristics of PDE intersect $\sim$ a shock develops)

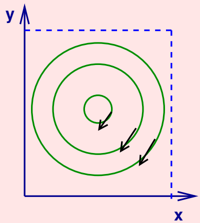


Transformation vs. grid [4]

Example 4:

consider the PDE $u_t = -2\pi(y - \frac{1}{2})u_x + 2\pi(x - \frac{1}{2})u_y$. MoC defines a transformation $(x(\xi, \eta, \theta), y(\xi, \eta, \theta), t = \theta)$ that must satisfy $\frac{\partial x}{\partial \theta} = 2\pi(y - \frac{1}{2})$, $\frac{\partial y}{\partial \theta} = -2\pi(x - \frac{1}{2})$, $\frac{\partial u}{\partial \theta} = 0$.

$\Rightarrow (x - \frac{1}{2})^2 + (y - \frac{1}{2})^2 = c^2$ (circles around $(\frac{1}{2}, \frac{1}{2})$)
The grid follows these trajectories $\Rightarrow$ grid distortion after some time (computations break down)



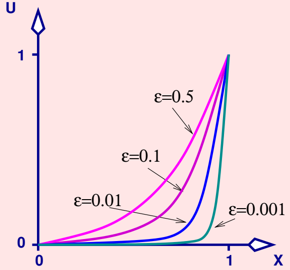
HOW TO CHOOSE THE TRANSFORMATION (GRID)??

A simple boundary value problem [0]

Consider the following BV-model:

$$\epsilon u_{xx} - u_x = 0, \quad u(0) = 0, \ u(1) = 1$$

with exact solution $$u^*(x) = \frac{e^{\frac{x}{\epsilon}} - 1}{e^{\frac{1}{\epsilon}} - 1}$$



A simple boundary value problem [1a]

Numerical approximation (idea 1):

$$\epsilon \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - \frac{u_{i+1} - u_{i-1}}{2\Delta x} = 0, \; i = 1 : N-1$$

The exact num. sol.: $u_i = \frac{\left(\frac{1+P_e}{1-P_e}\right)^i - 1}{\left(\frac{1+P_e}{1-P_e}\right)^N - 1}$ $\left(P_e := \frac{\Delta x}{2\epsilon},\; \Delta x = \frac{1}{N}\right)$

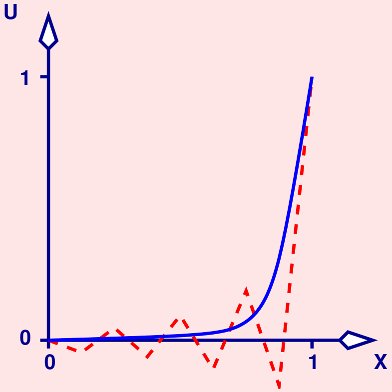
⋆ for $N < \frac{1}{2\epsilon} \rightsquigarrow P_e > 1$: numerical solution *oscillates*
⋆ for $N > \frac{1}{2\epsilon} \rightsquigarrow 0 < P_e < 1$: *monotone* numerical values

$0 < \epsilon \ll 1 \Longrightarrow N \gg 1$ (inefficiency of numerical process...)

⋆ The numerical error behaves like: $\mathcal{O}(\Delta x^2) = \mathcal{O}(\frac{1}{N^2})$

A simple boundary value problem [1b]

Numerical approximation (idea 1):



A simple boundary value problem [2a]

Numerical approximation (idea 2):

$$\epsilon \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} - \frac{u_i - u_{i-1}}{\Delta x} = 0, \;\; i = 1 : N-1$$

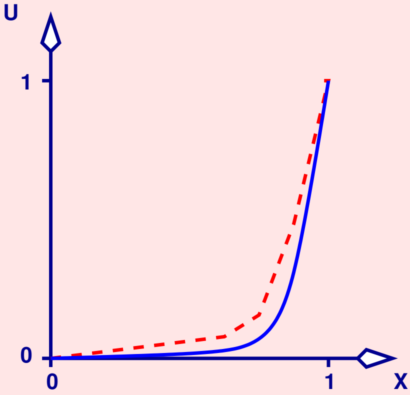
The exact num. sol: $u_i = \dfrac{(1+P_e)^i - 1}{(1+P_e)^N - 1}$

- $\star$ $1 + P_e > 1 \Longrightarrow u_{i+1} > u_i \; \forall i$ (*monotone* numerical solution)
- $\star$ Unfortunately, the error behaves as: $\mathcal{O}(\Delta x) = \mathcal{O}(\frac{1}{N})$
- $\star$ Also, extra numerical damping ("diffusion") is introduced:

$$\frac{u_i - u_{i-1}}{\Delta x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{\Delta x}{2} \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

A simple boundary value problem [2b]

Numerical approximation (idea 2):



A simple boundary value problem [3a]

Numerical approximation (idea 3):

define $v(\xi) := u(x(\xi))$ and a transformation $x \longmapsto \xi \in [0,1]$; then the BV-problem becomes

$$\frac{\epsilon}{x_\xi}\left[\frac{v_{\xi\xi}x_\xi - v_\xi x_{\xi\xi}}{x_\xi^2}\right] - \frac{v_\xi}{x_\xi} = 0$$

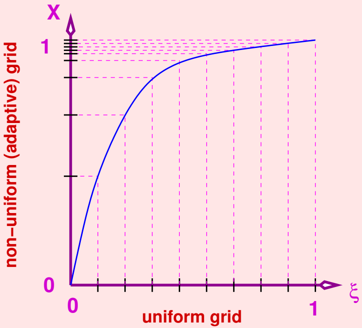
Suppose that $v(\xi) = \xi$ and assume $x_\xi > 0$, then

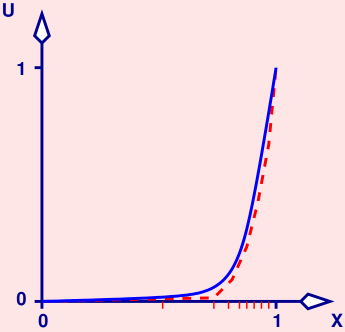
$$\epsilon x_{\xi\xi} + x_\xi^2 = 0, \quad x(0) = 0, \ x(1) = 1$$

with exact solution $x^*(\xi) = \epsilon \ln(\xi(e^{\frac{1}{\epsilon}} - 1) + 1)$

A simple boundary value problem [3b]

Numerical approximation (idea 3):





A simple boundary value problem [3c]

Numerical approximation (idea 3):

1. this particular mapping satisfies $\boxed{x_\xi u_x = 1}$, since $u_x = \frac{v_\xi}{x_\xi}$ and $v(\xi) = \xi \Rightarrow v_\xi = 1$.

2. $x_\xi \sim \frac{1}{\text{grid point concentration}}$

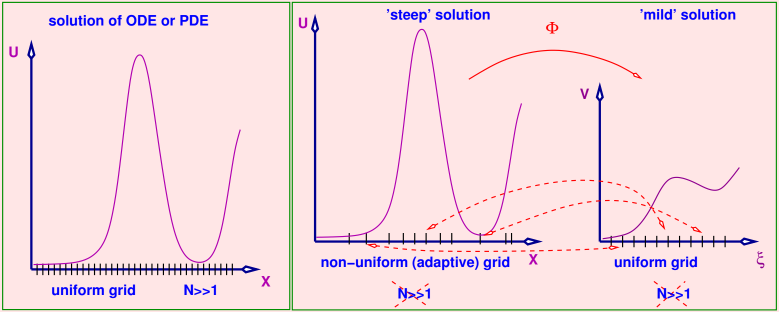
3. from 1. & 2.: where u_x *large* $\rightsquigarrow$ x_ξ *small*, i.e., grid points are concentrated in boundary layer

4. could use this principle for other models as well(!):

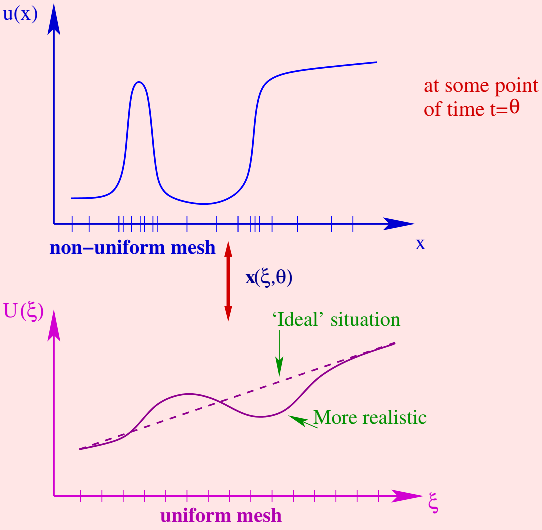
$$\boxed{x_\xi \, \omega = 1}$$

where $\omega > 0$ is a 'monitor' function

Adaptive grids in terms of coordinate transformations [1]



Adaptive grids in terms of coordinate transformations [2]



The equidistribution principle [1]

What is equidistribution?

We want to "equally distribute" a positive definite weight or monitor function ω on a non-uniform grid

Ideally: $\omega \sim$ some measure of the numerical error

choose or compute a grid

$$x_L = x_0 < x_1 < x_2 < \ldots < x_{N-1} < x_N = x_R$$

such that the contribution to the 'error' from each subinterval (x_{i-1}, x_i) is the same

The equidistribution principle [2]

The basic principle reads:

$$\Delta x_i \, \omega_i = c, \quad i = 0, \ldots, N-1$$

with $x_0 = x_L, \; x_N = x_R, \quad \Delta x_i := x_{i+1} - x_i$
which is a discrete version of (applying the midpoint rule):

$$\int_{x_i}^{x_{i+1}} \omega dx = c, \quad i = 0, \ldots, N-1$$

The constant c is determined from:

$$\int_{x_L}^{x_R} \omega dx = \int_{x_0}^{x_1} \omega dx + \int_{x_1}^{x_2} \omega dx + \ldots + \int_{x_{N-1}}^{x_N} \omega dx = c + c + \ldots + c \;\; (N \text{ times}),$$

giving $c = \frac{1}{N} \int_{x_L}^{x_R} \omega dx$.

The equidistribution principle [3]

We obtain:

$$\int_{x_i}^{x_{i+1}} \omega dx = \frac{1}{N} \int_{x_L}^{x_R} \omega dx, \quad i = 0, ..., N-1,$$

which means that the monitor function ω is equally distributed over all subintervals.

The main idea behind this principle:

grid cells Δx_i are small where ω_i is large, and vice versa, *since their product is constant*.

The equidistribution principle [4]

The *discrete* formulation:

$$\Delta x_i \; \omega_i = c$$

can also be interpreted as an approximation to the problem

$$\boxed{x_\xi \omega = c, \quad 0 < \xi < 1}$$

or, taking the ξ-derivative, to the boundary-value problem

$$\boxed{(\omega x_\xi)_\xi = 0, \quad x(0) = x_L, \quad x(1) = x_R}$$

The equidistribution principle [5]

Note that

since $\frac{dx}{d\xi} = \frac{1}{\frac{d\xi}{dx}}$, we find

$$\frac{d\xi}{dx} = c\,\omega, \quad x_L < x < x_R,\ \xi(x_L) = 0,\ \xi(x_R) = 1$$

We then obtain

$$1 = 1 - 0 = \xi(x_R) - \xi(x_L) = \int_{x_L}^{x_R} \frac{d\xi}{dx}\,dx = c\int_{x_L}^{x_R} \omega dx,$$

so that $c = \frac{1}{\int_{x_L}^{x_R} \omega dx} \Rightarrow \frac{d\xi}{dx} = \frac{\omega}{\int_{x_L}^{x_R} \omega dx}$

The equidistribution principle [6]

Integration of

$$\frac{d\xi}{dx} = \frac{\omega}{\int_{x_L}^{x_R} \omega d\bar{x}}$$

defines the inverse transformation

$$\xi(x) = \int_{x_L}^{x} \frac{\omega}{\int_{x_L}^{x_R} \omega d\bar{x}} d\bar{x} = \frac{\int_{x_L}^{x} \omega d\bar{x}}{\int_{x_L}^{x_R} \omega d\bar{x}}$$

Note that

$$\xi_x = \frac{1}{x_\xi}$$

represents the 'grid point density' of the transformation

The equidistribution principle [7]

Regularity of the transformation

$$\frac{dx}{d\xi}\omega = c = \frac{x_R - x_L}{\int_0^1 \omega d\bar{\xi}}$$

For $\omega > 0 \Rightarrow c > 0$, we have $\frac{dx}{d\xi} > 0$ (of course, $x_R - x_L > 0$). The Jacobian of the transformation is given by $\frac{dx}{d\xi} > 0 \Rightarrow$
transformation is non-singular.

In terms of the grid points, $\Delta x_i \omega_i = c > 0 \Rightarrow \Delta x_i > 0$: the grid points do not cross!

The equidistribution principle [8]

Variational formulation:

Consider the ‘grid-energy’

$$\mathcal{E} = \int_0^1 \omega x_\xi^2 d\xi$$

Minimizing this functional via the Euler-Lagrange equation:

$$\frac{d}{d\xi}\left(\frac{\partial \mathcal{F}}{\partial x_\xi}\right) - \frac{\partial \mathcal{F}}{\partial x} = 0 \quad \text{with} \quad \mathcal{F} = \mathcal{F}(x, x_\xi) = \omega(\xi) x_\xi^2 \quad \text{gives:}$$

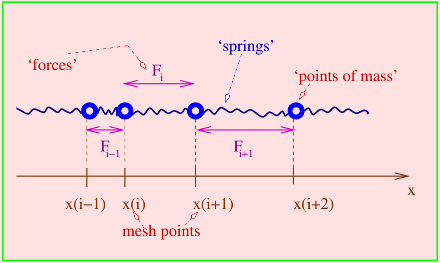
$$\frac{d}{d\xi}(2\omega x_\xi) - 0 = 0 \Leftrightarrow \boxed{\frac{d}{d\xi}[\omega \frac{dx}{d\xi}] = 0}$$

which is equivalent to the differential formulation (BV-problem)

The equidistribution principle [9]

The ‘grid-energy’

can be taken to represent the energy of a system of springs with spring constants ω spanning each interval.
The non-uniform grid point distribution resulting from the equidistribution principle thus represents the equilibrium state of the spring system, i.e., the state of minimum energy.

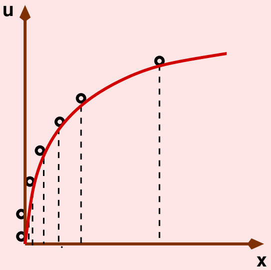


The equidistribution principle [10]

How to choose ω? (choice 1)

$$\omega = u_x \;\Rightarrow x_\xi \omega = x_\xi u_x = x_\xi \frac{v_\xi}{x_\xi} = v_\xi = c$$

The grid points x_i adjust in such a way that the same change in the solution u occurs over each grid interval (x_{i-1}, x_i);
disadvantage: $(u_x \downarrow 0 : \; \Delta x_i \to \infty)$

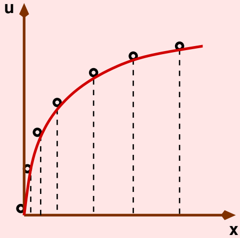


The equidistribution principle [11]

How to choose ω? (choice 2)

$\omega = \sqrt{1+u_x^2}$: an increment of *arclength* ds on the solution curve $u(x)$ is given by $ds^2 = dx^2 + du^2 = (1+u_x^2)dx^2 \Rightarrow$
$\omega = s_x \;\Rightarrow x_\xi s_x = x_\xi \frac{s_\xi}{x_\xi} = s_\xi = c$. Note: $u_x \downarrow 0 \Rightarrow \Delta x_i \to \frac{1}{N}$

The grid point distribution is now such that the same increment in arclength in the solution occurs over each subinterval



Can we expect problems with this approach?