Lecture 12; Part II

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Numerical Methods for Time-Dependent PDEs, Spring 2024

Contents of part 2

Smoothed equidistribution and applications:

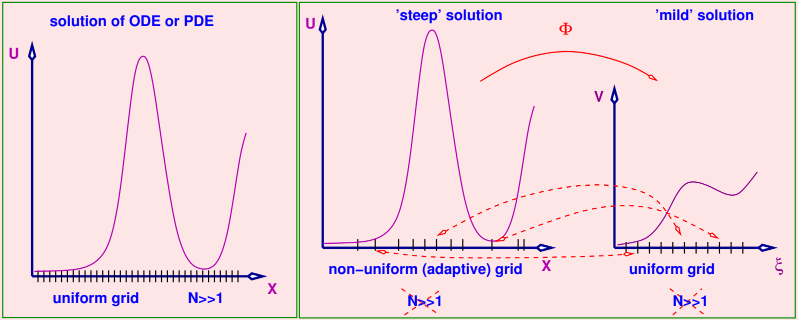
- Grid distributions, local truncation error & (un)stable grid motion

- (local) quasi-uniformity

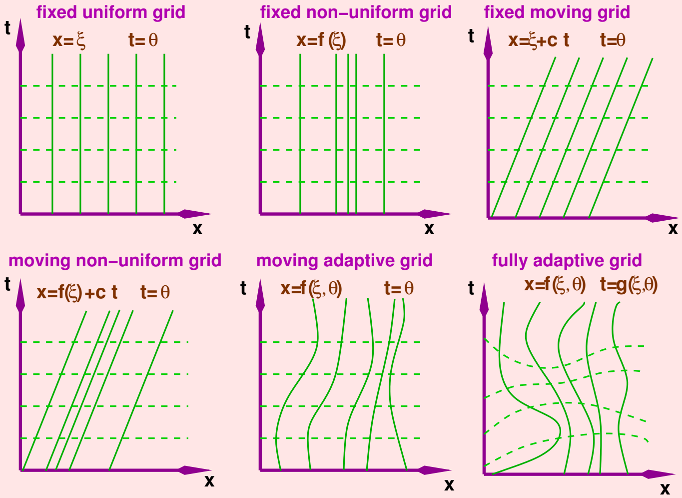
- Smoothness in space and time

- 1D applications from chemistry, hydrology, magneto-hydrodynamics, ...

Adaptive grids in terms of coordinate transformations



Different types of mappings based *moving* adaptive grids



Recall: the equidistribution principle [1]

The *equidistribution principle* in 1D is:

$$(\omega x_\xi)_\xi = 0, \quad x(0) = x_l, \quad x(1) = x_r$$

An explicit formula for the inverse transformation can be derived:

$$1 = \xi(x_r) - \xi(x_l) = \int_{x_l}^{x_r} \xi_x \, d\bar{x} = c \int_{x_l}^{x_r} \omega \, d\bar{x} \Rightarrow \xi_x = \frac{\omega(x)}{\int_{x_l}^{x_r} \omega \, d\bar{x}}$$

and integrating once more gives

$$\xi(x) = \frac{\int_{x_l}^{x} \omega(\bar{x}) \, d\bar{x}}{\int_{x_l}^{x_r} \omega(\bar{x}) \, d\bar{x}}$$

Recall: equidistribution principle [2]

Discrete formulation:

$$\Delta x_i \; \omega_i = \text{constant} \Rightarrow \Delta x_i > 0 \quad \forall i \quad \rightsquigarrow \mathcal{J} := x_\xi > 0$$

(1D transformation is non-singular, if $\omega > 0$)

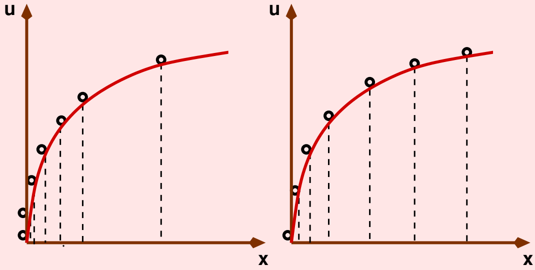
The monitor function ω is *equally distributed* over all subintervals

$$\int_{x_i}^{x_{i+1}} \omega \; d\bar{x} = \frac{1}{N} \int_{\Omega_p} \omega \; d\bar{x}$$

Recall: the equidistribution principle [3]

1) $\omega = u_x \ \rightsquigarrow\ u_\xi = \text{constant}$
$(u_x \downarrow 0:\ \ \Delta x_i \to \infty)$

2) $\omega = \sqrt{1+u_x^2}; \quad ds^2 = dx^2 + du^2 = (1+u_x^2)dx^2$
$\Rightarrow \omega = s_x \ \rightsquigarrow\ s_\xi = \text{constant}$ $(u_x \downarrow 0:\ \ \Delta x_i \to \frac{1}{N})$

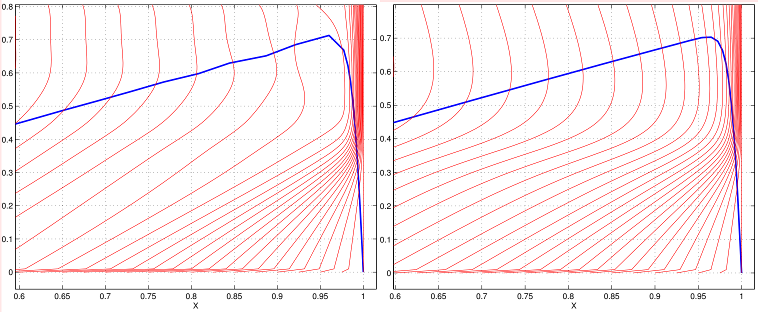


unsmooth vs. *smooth* grid

Burgers' equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0.005\frac{\partial^2 u}{\partial x^2}, \quad x \in [0,1]$$

with $u(x,0) = \sin(\pi x), \; u(0,t) = u(1,t) = 0$

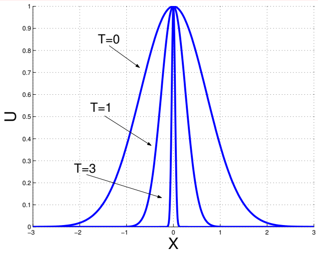


A linear hyperbolic PDE [1]; *smoothed* equidistribution

$$\frac{\partial u}{\partial t} - x\frac{\partial u}{\partial x} = 0, \quad x \in [-3, 3]$$

with exact solution

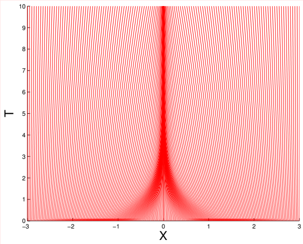
$$u(x,t) = e^{-(e^t x)^2}$$

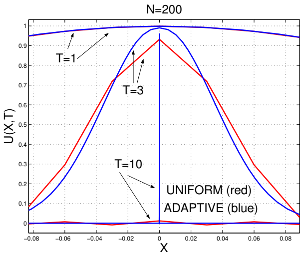


method of characteristics: $\begin{cases} \dot{x} = -x \\ \dot{u} = 0 \end{cases}$

A linear hyperbolic PDE [2]; *smoothed* equidistribution

N	$\|\|e\|\|_\infty$: *Un.* $t = 5$	*Ad.* $t = 5$	*Un.* $t = 10$	*Ad.* $t = 10$
100	0.669504	0.050343	0.993392	0.144466
200	0.506568	0.018615	0.988101	0.040614
400	0.322038	0.008071	0.978686	0.017416
800	0.161977	0.003626	0.962241	0.008049
1600	0.060010	0.001640	0.934068	0.003819





Another PDE example [1]; *smooth* vs. *unsmooth* grid

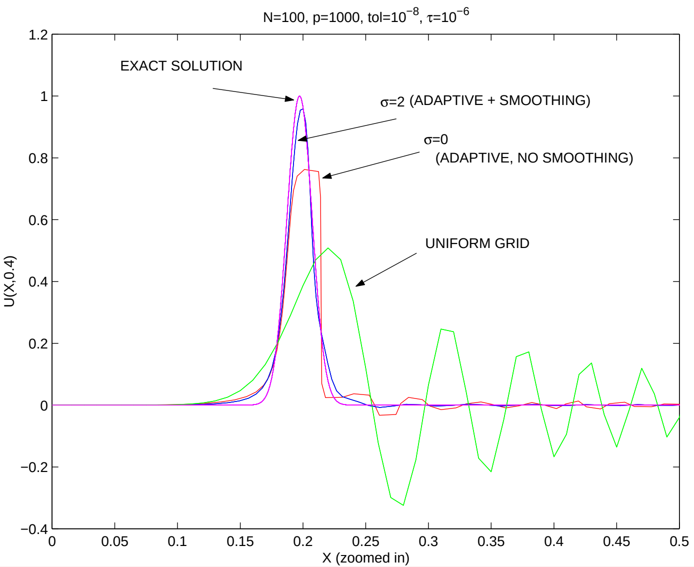
$$\frac{\partial u}{\partial t} + 4\cos(4\pi t)\frac{\partial u}{\partial x} = 0$$

⋆ An exact solution of this hyperbolic PDE is

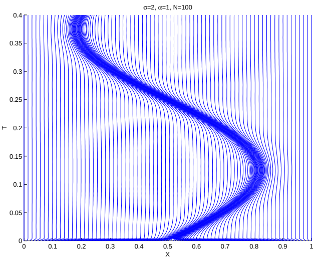
$$u^*(x,t) = \sin^{1000}(\pi(x - \frac{1}{\pi}\sin(4\pi t)))$$

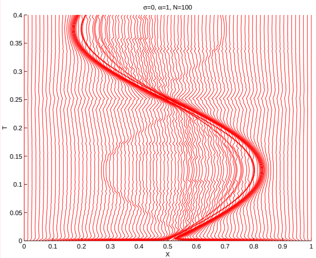
⋆ It describes an *extremely sharp* pulse that *moves periodically* in the time direction, from left to right and backwards again through the spatial domain

Another PDE example [2]; *smooth* vs. *unsmooth* grid



Another PDE example [3]; *smooth* vs. *unsmooth* grid



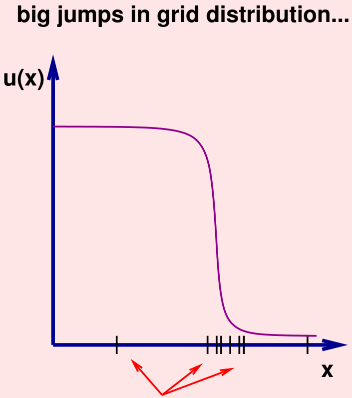


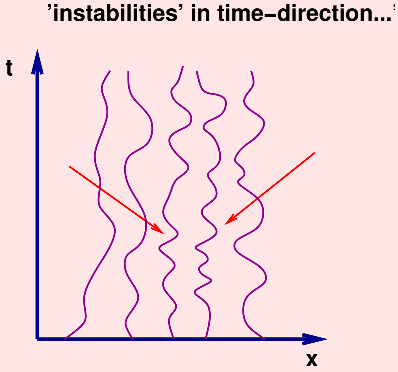
Another PDE example [4]; *smooth* vs. *unsmooth* grid

The maximum error at $t = 0.4$:

N	*uniform*	*unsmooth equid.*	*smooth equid.*
50	0.721312	0.624699	0.387192
100	0.577044	0.432729	0.116723
200	0.509914	0.274196	0.033135
400	0.327693	0.142711	0.025296
800	0.109807	0.072737	0.017410
1600	0.027250	*****	0.011549

So, what can still go wrong (*without* smoothing)???





Can we quantify these two aspects?

Yes, in terms of

- *local truncation errors* on non-uniform grids

and

- *unsmoothness of a time-dependent grid* based on *pure* equidistribution.

The grid size ratio and the truncation error [1]

Define the 'grid size ratio' ('local stretching factor'):

$$r := \frac{x_i - x_{i-1}}{x_{i+1} - x_i} := \frac{\Delta x_{i-1}}{\Delta x_i} := \frac{q}{p}$$

The truncation error T for the central finite difference approximation $u_{x,i} \approx \frac{u_{i+1} - u_{i-1}}{p+q}$ is then given by

$$\begin{aligned}
&= -\tfrac{p^2-q^2}{2(p+q)} u_{xx,i} - \tfrac{p^3+q^3}{6(p+q)} u_{xxx,i} + \ldots \\
&= -\tfrac{1}{2} u_{xx,i}(1-r)\Delta x_i - \tfrac{1}{6} u_{xxx,i}(1 - r + r^2)\Delta x_i^2 + \ldots \\
&= \tfrac{\Delta\xi^2}{6}(3x_{\xi\xi,i} u_{xx,i} + x_\xi^2 u_{xxx,i}) + \mathcal{O}(\Delta\xi^4) \\
&= \Delta x_i^2 (\tfrac{1}{2} \tfrac{x_{\xi\xi,i}}{x_{\xi,i}} u_{xx,i} + \tfrac{1}{6} u_{xxx,i}) + \mathcal{H.O.T.}
\end{aligned}$$

The grid size ratio and the truncation error [2]

We see that for $r = 1$ (a uniform grid) we have a *second-order* approximation:

$$T = -\frac{\Delta\xi^2}{6} u_{xxx,i} + \mathcal{O}(\Delta\xi^4)$$

For the non-uniform grid, $r \neq 1$, the approximation is of *second order*, if $r = 1 + \mathcal{O}(\Delta x_i)$.

Since

$$r = \frac{x_{\xi,i}\Delta\xi - \frac{1}{2}\Delta\xi^2 x_{\xi\xi,i}}{x_{\xi,i}\Delta\xi + \frac{1}{2}\Delta\xi^2 x_{\xi\xi,i}} + \mathcal{H.O.T.} = 1 - \Delta x_i \frac{x_{\xi\xi,i}}{x_{\xi,i}^2} + \mathcal{H.O.T.}$$

we can conclude that $\frac{x_{\xi\xi,i}}{x_{\xi,i}^2} = \mathcal{O}(1) \Leftrightarrow r = 1 + \mathcal{O}(\Delta x_i)$.

The grid size ratio and the truncation error [3]

If the ratio $\frac{x_{\xi\xi,i}}{x_{\xi,i}^2}$ is too big, then $r \neq \mathcal{O}(1)$ and this influences the order of the truncation error.

Grids with $r = 1 + \mathcal{O}(\Delta x_i)$ are called 'quasi-uniform'.

Such grids (in terms of the transformation: $\frac{x_{\xi\xi,i}}{x_{\xi,i}^2} = \mathcal{O}(1)$) are 'smooth' enough and will not change greatly between adjacent intervals.

How to adjust the equidistribution principle to guarantee this, we will see further on.

Equidistribution and instabilities in time [1]

If we differentiate the equidistribution relation

$$\int_{x_L}^{x_i(t)} \omega dx = \frac{i}{N} \int_{x_L}^{x_R} \omega dx := \frac{i}{N} \omega(t), \quad i = 1, \ldots, N$$

with respect to time t we obtain

$$\omega(x_i, t)\dot{x}_i + \int_{x_L}^{x_i} \frac{\partial \omega}{\partial t}(x, t) dx = \frac{i}{N} \dot{\omega}(t), \quad i = 1, \ldots, N.$$

Introducing small perturbations δx_i on the grid points x_i and using Taylor expansions for $\omega(x_i + \delta x_i, t)$ and $\int_{x_L}^{x_i + \delta x_i} \frac{\partial \omega}{\partial t} dx$ we get

$$\omega(x_i, t)\dot{x}_i + \frac{\partial \omega}{\partial x} \delta x_i \dot{x}_i + \omega(x_i, t) \delta \dot{x}_i + \int_{x_L}^{x_i} \frac{\partial \omega}{\partial t} dx + \frac{\partial \omega}{\partial t} \delta x_i + \mathcal{H}.\mathcal{O}.\mathcal{T}. = \frac{i}{N} \dot{\omega}(t)$$

Equidistribution and instabilities in time [2]

After linearization follows

$$\omega(x_i,t)\delta\dot{x}_i + \frac{\partial\omega}{\partial x}\delta x_i\dot{x}_i + \frac{\partial\omega}{\partial t}\delta x_i = 0.$$

This is equivalent with $\frac{d}{dt}[\omega(x_i(t),t)\delta x_i] = 0$ and integrating once gives

$$\omega(x_i(t),t)\delta x_i(t) = \text{CONSTANT} = \omega(x_i(0),0)\delta x_i(0)$$

and therefore $\delta x_i(t) = \frac{\omega(x_i(0),0)}{\omega(x_i(t),t)}\delta x_i(0)$. From this expression we see that, if $\frac{\omega(x_i(0),0)}{\omega(x_i(t),t)}$ becomes > 1, the adaptive grid in equidistribution may become *unstable*. This may be prevented by adding a small 'delay'-term to the equidistribution principle.

Smoothed equidistribution in space and time [1]

An important inequality is therefore

$$\frac{1}{K} \leq r \leq K, \quad K = \mathcal{O}(1)$$

Re-write the EP $\Delta x_i \omega_i = c(t)$ in terms of 'point concentrations' $n_i := \frac{1}{\Delta x_i}$:

$$n_i = \bar{c}(t)\omega_i, \quad \forall i$$

Define

$$\breve{\omega}_i = \sum_{j=0}^{N} \omega_j \left(\frac{\sigma}{\sigma+1}\right)^{|i-j|}, \quad \sigma > 0, \quad \omega > 0$$

and *replace* the EP by

$$n_i = \bar{c}(t)\breve{\omega}_i, \quad \forall i$$

Smoothed equidistribution in space and time [2]

Lemma: From $n_i = \bar{c}(t)\breve{\omega}_i, \ \forall i$, it follows $\Rightarrow \frac{\sigma}{\sigma+1} \leq \frac{n_i}{n_{i-1}} \leq \frac{\sigma+1}{\sigma}, \ \forall i$
[the magnitude of ω does not play a role at all! Note that, if $\sigma = \mathcal{O}(1)$ then $r = \frac{n_i}{n_{i-1}} = \mathcal{O}(1)$].

Define $\tilde{n}_i := n_i - \sigma(\sigma+1)(n_{i+1} - 2n_i + n_{i-1}) = \tilde{c}(t)\omega_i, \ \forall i$ with $n_0 = n_1, \ n_{N-1} = n_N$.

Then the solution of this system of equations is given by

$$n_i = \tilde{c}\ C_+(\frac{\sigma+1}{\sigma})^i + \tilde{c}\ C_-(\frac{\sigma}{\sigma+1})^i + \tilde{c}\sum_{j=1}^{N-1}(\frac{\sigma}{\sigma+1})^{|i-j|}$$

for some constants C_+ and C_- that depend on the boundary values.

Smoothed equidistribution in space and time [3]

Lemma: This solution n_i has the property

$$\frac{\sigma}{\sigma+1} \leq \frac{n_i}{n_{i-1}} \leq \frac{\sigma+1}{\sigma},\ \forall i$$

.

Instead of $n_i = \bar{c}(t)\breve{\omega}_i$ which is equivalent with $\tilde{n}_i = \tilde{c}(t)\omega_i$ we set

$$\tilde{n}_i(t) + \tau_s \frac{d}{dt}\tilde{n}_i(t) = \tilde{c}(t)\omega_i,\ \forall i$$

with boundary conditions $n_0 = n_1,\quad n_{N-1} = n_N,\ \forall t.$

Note that the solution of this $ODE - system$ can be obtained in terms of an integral equation:

$$\tilde{n}_i(t) = \exp(-t/\tau_s)[\tilde{n}_i(0) + \int_0^t \tau_s^{-1}\exp(s/\tau_s)c(s)\omega_i(s)ds],\ t \geq 0,\ \forall i.$$

Smoothed equidistribution in space and time [4]

If we apply, for instance, Euler-Backward to the ODE-system we can make the following observations with respect to τ_s:

$\tau_s \to 0: \quad \tilde{n}_i^{(n+1)} \approx c^{(n+1)} \omega_i^{(n+1)} \ \forall i$ no time smoothing

$\tau_s \gg \Delta t: \quad \tilde{n}_i^{(n+1)} \approx \tilde{n}_i^{(n)} \ \forall i$ too much smoothing $\Rightarrow$ no grid adaptation

$\tau_s = \mathcal{O}(\Delta t): \quad \tilde{n}_i^{(n+1)} \approx \frac{1}{2} \tilde{n}_i^{(n)} + \frac{1}{2} c^{(n+1)} \omega_i^{(n+1)} \ \forall i$ (use old values as well to adapt grid)

Lemma: For $\sigma = \tau_s = 0$, i.e., no smoothing at all: $n_i = \bar{c}(t) \omega_i)$ and $\omega > 0 \Rightarrow n_i > 0, \ \forall i$.

Smoothed equidistribution in space and time [5]

The case $\tau_s = 0,\ \sigma \neq 0$:
We have seen that $\tilde{n}_i = \tilde{c}\omega_i \Leftrightarrow n_i = \bar{c}\breve{\omega}_i\ \forall i\ \ (\breve{\omega}_i > 0)$. From the previous Lemma follows $n_i > 0,\ \forall i$ (simply replace ω_i by $\breve{\omega}_i$).

Lemma: If n_i is the solution given by

$$n_i = \tilde{c}\ C_+(\frac{\sigma+1}{\sigma})^i + \tilde{c}\ C_-(\frac{\sigma}{\sigma+1})^i + \tilde{c}\sum_{j=1}^{N-1}(\frac{\sigma}{\sigma+1})^{|i-j|}$$

then, because $n_i > 0 \Rightarrow \tilde{n}_i > 0\ \forall i$.

The case $\tau_s \neq 0,\ \sigma = 0:\ \ n_i + \tau_s \frac{d}{dt} n_i = \hat{c}(t)\omega_i$.

Lemma: $n_i(0) > 0,\ \ \forall i \Rightarrow n_i(t) > 0\ \forall i\ \ \forall t \geq 0$.

Smoothed equidistribution in space and time [6]

The case $\tau_s \neq 0, \ \sigma \neq 0$:
We then use:

$$\tilde{n}_i(t) + \tau_s \frac{d}{dt}\tilde{n}_i(t) = \tilde{c}(t)\omega_i, \ \forall i$$

Lemma: The solution n_i (in terms of $\tilde{n}_i$) is a linear combination of $\tilde{n}_i$-values with only positive coefficients (i.e. $\tilde{n}_i > 0 \Rightarrow n_i > 0$).

Theorem:
I) $\Delta x_i(0) > 0 \ \ \forall i \Rightarrow \Delta x_i(t) > 0 \ \forall i, \ \forall t \geq 0.$
II) $\frac{\sigma}{\sigma+1} \leq \frac{\Delta x_{i+1}(t)}{\Delta x_i(t)} \leq \frac{\sigma+1}{\sigma}, \ \forall i, \ \forall t \geq 0.$

An adaptive grid PDE [1]

Consider time-dependent PDE:

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \beta \frac{\partial u}{\partial x} + s(u, x, t)$$

Apply transformation:

$$\begin{aligned} x &= x(\xi, \theta) \\ t &= t(\xi, \theta) = \theta \\ \mathcal{J} &:= x_\xi \end{aligned}$$

$$\Longrightarrow U_\theta - \frac{1}{\mathcal{J}} x_\theta U_\xi = \frac{\epsilon}{\mathcal{J}} [\frac{1}{\mathcal{J}} U_\xi]_\xi - \frac{\beta}{\mathcal{J}} U_\xi + s(x, U, \theta)$$

Semi-discretization (uniform in ξ):

$$\dot{U}_i - \frac{U_{i+1} - U_{i-1}}{x_{i+1} - x_{i-1}} (\dot{x}_i - \beta) = \epsilon \frac{\frac{U_{i+1} - U_i}{x_{i+1} - x_i} - \frac{U_i - U_{i-1}}{x_i - x_{i-1}}}{\frac{1}{2}(x_{i+1} - x_{i-1})} + s_i$$

An adaptive grid PDE [2]

Let the transformation be the solution of:

$$[(\mathcal{S}(x_\xi) + \tau_s x_{\xi\theta})\omega]_\xi = 0$$

$\tau_s \Rightarrow$ temporal smoothing parameter

weight function: $\omega = \sqrt{1 + \sum_k \alpha_k (U_{x,k})^2}$

$\alpha_k \Rightarrow$ adaptivity parameters

The smoothing operator $\mathcal{S}$ is defined by:

$$\mathcal{S} = \mathcal{I} - \sigma(\sigma+1)(\Delta\xi)^2 \frac{\partial^2}{\partial\xi^2}$$

$\sigma \Rightarrow$ spatial smoothing parameter

An adaptive grid PDE [3]

Some properties of the grid:

i)

$$\mathcal{J} = x_\xi > 0 \quad \forall\ \theta \in [0, T]$$

In discretized form ($\Delta\xi$ is constant):

$$\Delta x_i(\theta) > 0 \quad \forall\ \theta \in [0, T]$$

$\Rightarrow$ No ‘node-crossing’ possible!

ii)

$$\left|\frac{x_{\xi\xi}}{x_\xi}\right| \leq \frac{1}{\sqrt{\sigma(\sigma+1)\Delta\xi}}$$

In discretized form:

$$\frac{\sigma}{\sigma+1} \leq \frac{\Delta x_{i+1}(\theta)}{\Delta x_i(\theta)} \leq \frac{\sigma+1}{\sigma} \quad \forall\ \theta \in [0, T]$$

$\Rightarrow$ ‘Local quasi-uniformity’!

An adaptive grid PDE [4]

iii)

$$\tau_s = \sigma = 0 \quad \Rightarrow \quad x_\xi \, \omega = \text{constant} \quad \forall \, \theta \in [0, T]$$

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

In discretized form:

$$\Delta x_i \cdot \omega_i = \text{constant} \quad \forall \, \theta \in [0, T]$$

$\Rightarrow$ Equidistribution of arc-length monitor

iv)

$$0 < \tau_s \leq 10^{-3} \times \text{timescale in PDE model}$$

$$\sigma = \mathcal{O}(1) \quad (\sigma = 2 \ \text{ suffices in general})$$

$$\alpha_k = \mathcal{O}(1) \quad \text{depends on } x \text{ and } U_k \text{ scales}$$

An adaptive grid PDE [5]

Semi-discretization of the adaptive grid PDE:

$$[\tilde{\Delta}x_{i+1} + \tau_s \frac{\mathrm{d}\Delta x_{i+1}}{\mathrm{d}\theta}]\omega_{i+1} - [\tilde{\Delta}x_i + \tau_s \frac{\mathrm{d}\Delta x_i}{\mathrm{d}\theta}]\omega_i = 0$$

where $\tilde{\Delta}x_i = \Delta x_i - \sigma(\sigma+1)(\Delta x_{i+1} - 2\Delta x_i + \Delta x_{i-1})$

$\Rightarrow$ adaptive-grid ODE system:

$$\tau_s\ \mathcal{B}(\vec{X}, \vec{U}, \sigma, \alpha_k)\dot{\vec{X}} = \vec{\mathcal{H}}(\vec{X}, \vec{U}, \sigma, \alpha_k)$$

Coupled on semi-discretized PDE system $\Rightarrow$ large, stiff, banded, nonlinear ODE system [BDF-methods (order ≤ 5): DASSL]

Application: the Gray-Scott-model [1]

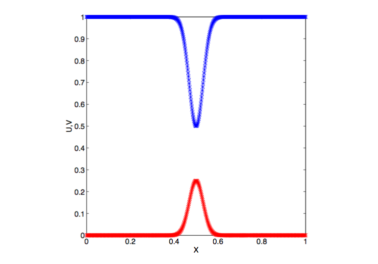
Pattern formation in ferrocyanide-iodate-sulphite reactions:

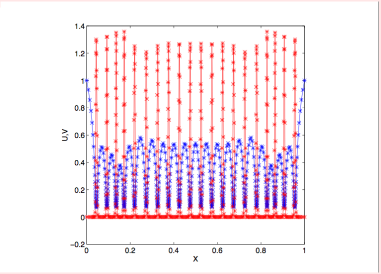
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - uv^2 + A(1-u)$$
$$\frac{\partial v}{\partial t} = 0.01\frac{\partial^2 v}{\partial x^2} + uv^2 - Bv$$

from:

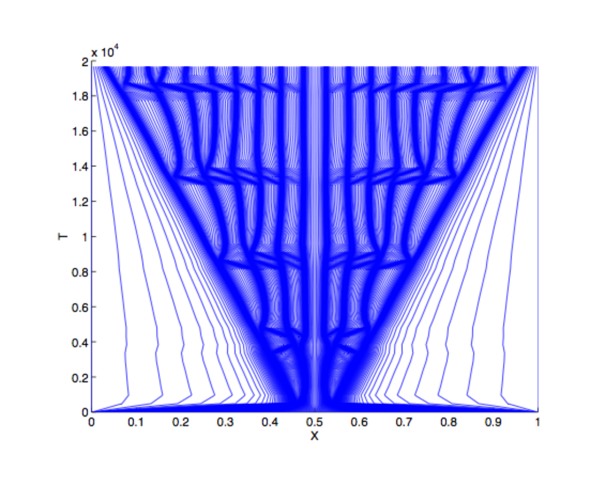
A. Doelman, T. J. Kaper and P. A. Zegeling
Pattern formation in the 1-D Gray-Scott model
Nonlinearity, V10, pp. 523-563, 1997

Application: the Gray-Scott-model [2]





Application: the Gray-Scott-model [3]



Application: Golden-Gate-bridge-model [1]

$$u_{tt} + u_{xxxx} + u^+ - 1 = 0 \quad \text{with } u^+ = \begin{cases} u, & u > 0 \\ 0, & u < 0 \end{cases}$$

The solution $u(x,t)$ represents the displacement of a beam from the unloaded state.

'Historical accounts of travelling wave behaviour in the Golden Gate Bridge in San Francisco motivated us to study this PDE'.

It can be re-written as $\boxed{\tilde{u}_t = \mathcal{A}\tilde{u}_{xx} + \mathcal{B}\tilde{u} + \mathcal{F}}$

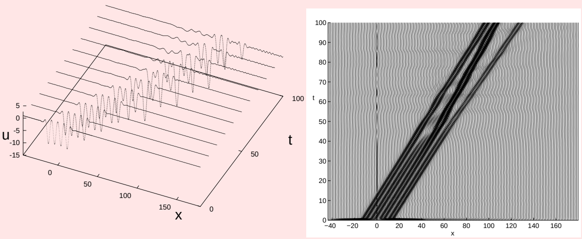
where $\tilde{u} := (u, v, w)^T, \; v = u_t, \; w = u_{xx}, \mathcal{F} = (0, u^+ - 1, 0)^T$ and

$$\mathcal{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

from Champneys, McKenna & Zegeling, *Nonl. Dynamics*, 21, pp. 31-53, 2000

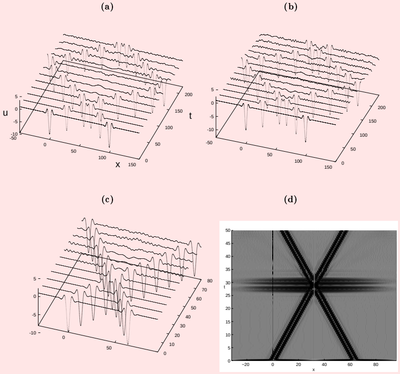
Application: Golden-Gate-bridge-model [2]

(a) (b)



(a) Solution and **(b)** the moving mesh method for the $\mathbf{4}(2,2,2)$ wave using the same initial data as in Figure 4. The data presented is for a run with 1501 grid points, a more accurate run with 2001 produced qualitatively the same a non-trivial task.

Application: Golden-Gate-bridge-model [3]



(a) Solution to (1) with the piecewise-linear term (2) using the fixed grid method showing the interaction of two primary waves with initial wave speeds $c = 1.1$ and -1.1. **(b)** The equivalent run for the exponential nonlinearity (4). **(c)** The same run as (b) using the moving grid method with 2001 grid points; and **(d)** motion of the grid (from a qualitatively identical run with 1001 grid points)

Application: a tumour angiogenesis model [1]

Angiogenesis: blood vessel development

$$b_t + ([\tfrac{3}{4}c_x]b)_x = 10^{-3}b_{xx} - 4b + 10^2 b(1-b)\max(0, c-0.2)$$
$$c_t = \delta c_{xx} - c - 10\frac{bc}{1+c}, \quad x \in [0,1]$$

b: density of endothelial cells (blood)
c: tumour angiogenesis factor (TAF)

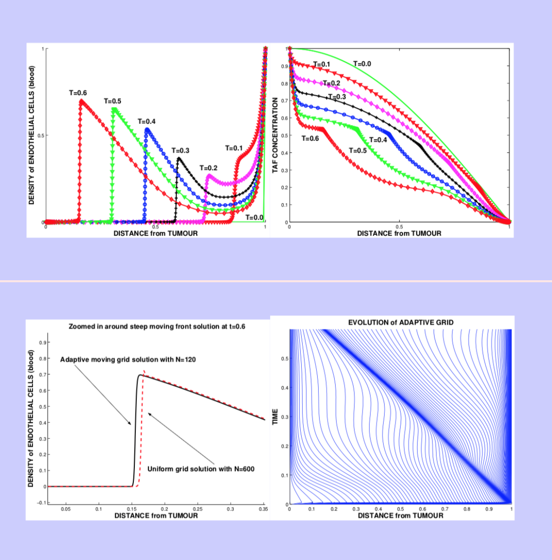
$$c(x,0) = \cos(\frac{1}{2}\pi x), \;\; b(x,0) = \begin{cases} 0, & \text{if } 0 \le x < 1 \\ 1, & \text{if } x = 1 \end{cases}$$

$$b(0,t) = 0, \;\; b(1,t) = 1, \;\; c(0,t) = 1, \;\; c(1,t) = 0$$

(numerical experiments with $\delta = 1$ and $\delta = 10^{-3}$)

from Chaplain & Stuart, 1993

Application: a tumour angiogenesis model [2]



Application: brine transport in a porous medium [1]

$$(n\rho)_t + (\rho q)_x = 0, \quad q = -\frac{k}{\mu}(p_x + \rho g)$$
$$(n\rho\omega)_t + (\rho\omega q + \rho J)_x = 0, \quad J = -\lambda|q|\omega_x$$

ω: salt concentration

the fluid density ρ satisfies the equation of state

$$\rho = \rho_0 e^{\beta(p-p_0)+\gamma\omega}$$

ICs and BCs:

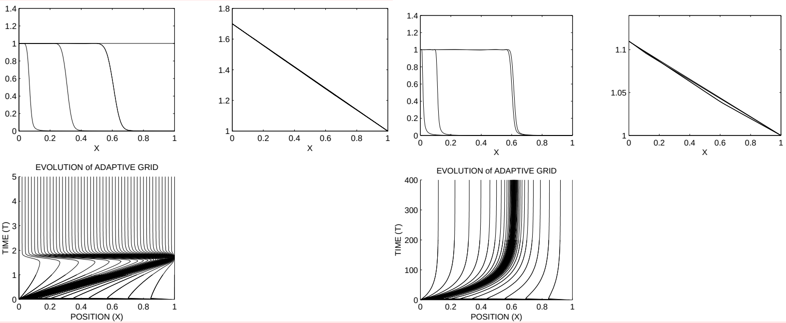
$$\omega(x,0) = 0,\ \omega(0,t) = \omega_0 > 0,\ \omega_x(1,t) = 0,\ x \in [0,L]$$

$$p(x,0) = p_0[(1-\frac{x}{L})p_{left} + \frac{x}{L}p_{right}]$$

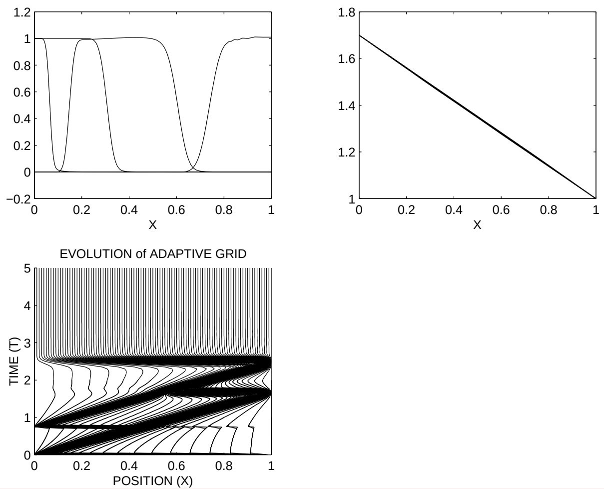
$$p(0,t) = p_0 p_{left},\ p(1,t) = p_0 p_{right}$$

from Zegeling, Verwer & v. Eijkeren, Int. J. Num. Methods in Fluids, 15, pp. 175-191, 1992

Application: brine transport in a porous medium [2]



Application: brine transport in a porous medium [3]



Application: an MHD-model in 1.75D [1]

$$\frac{\partial \rho}{\partial t} + \frac{\partial m_1}{\partial x} = 0 \qquad \bar{B}_1 = \text{constant} \qquad \mathbf{u} = \frac{\mathbf{m}}{\rho} \qquad \mathbf{B} = (\bar{B}_1, B_2, B_3)^T$$

$$\frac{\partial m_1}{\partial t} + \frac{\partial}{\partial x}\left(\frac{m_1^2}{\rho} - \bar{B}_1^2 + (\gamma - 1)\frac{\mathbf{m}^2}{2\rho} + (2-\gamma)\frac{\mathbf{B}^2}{2}\right) = 0$$

$$\frac{\partial m_2}{\partial t} + \frac{\partial}{\partial x}(m_1 v - \bar{B}_1 B_2) = 0 \qquad \frac{\partial m_3}{\partial t} + \frac{\partial}{\partial x}(m_1 w - B_1 B_3) = 0$$

$$\frac{\partial B_2}{\partial t} + \frac{\partial}{\partial x}(B_2 u - \bar{B}_1 v) = 0 \qquad \frac{\partial B_3}{\partial t} + \frac{\partial}{\partial x}(B_3 u - \bar{B}_1 w) = 0$$

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}\left[u\left(\gamma e - (\gamma - 1)\frac{\mathbf{m}^2}{2\rho} + (2-\gamma)\frac{\mathbf{B}^2}{2}\right) - \bar{B}_1 \mathbf{B}\cdot\mathbf{u}\right] = 0$$

$$e = \frac{p}{\gamma - 1} + \rho\frac{\mathbf{u}^2}{2} + \frac{\mathbf{B}^2}{2}$$

from A. van Dam & P.A. Zegeling 2005

Application: an MHD-model in 1.75D [2]

$$\gamma = \frac{5}{3}, \quad \bar{B}_1 \equiv 1, \quad \Omega = [0, 1000], \quad t \in [0, 80]$$

$$\rho|_{t=0} = \begin{cases} 0.5 & \text{for } x \in [0, 350] \\ 0.1 & \text{elsewhere} \end{cases}, \quad m_1|_{t=0} = 0$$

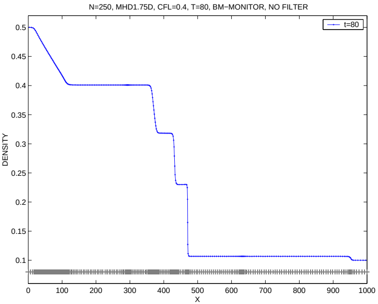
$$(m_2, m_3)|_{t=0} = \begin{cases} (0.5, 0.05) & \text{for } x \in [0, 350] \\ (0, 0) & \text{elsewhere} \end{cases}$$

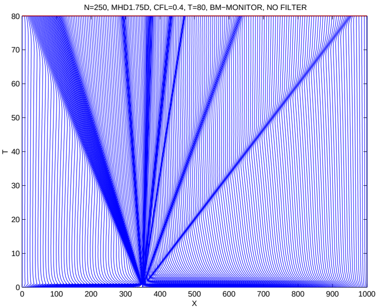
$$B_2|_{t=0} = \begin{cases} 2.5 & \text{for } x \in [0, 350] \\ 2 & \text{elsewhere} \end{cases}, \quad B_3|_{t=0} = 0$$

$$p|_{t=0} = \begin{cases} 1 & \text{for } x \in [0, 350] \\ 0.1 & \text{elsewhere} \end{cases}$$

Homogeneous Neumann BCs

Application: an MHD-model in 1.75D [3]





Application: heat flow of harmonic maps from surfaces [1]

Harmonic heat flow between the 2-disc D and the 2-sphere S:

$$u_t = \Delta u + |\nabla u|^2 u, \quad u(\mathbf{x},0) = \phi(\mathbf{x}), \quad u|_{\partial D} = \phi|_{\partial D}$$

Requiring spherical symmetry $\phi(\mathbf{x}) = [\frac{x}{|\mathbf{x}|}\sin(\psi(|\mathbf{x}|)), \cos(\psi(|\mathbf{x}|))]$, it can be shown that the solution must satisfy

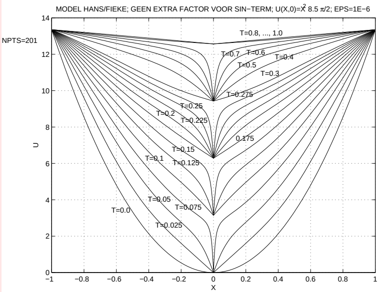
$$u(\mathbf{x},t) = [\frac{x}{|\mathbf{x}|}\sin(h(|\mathbf{x}|)), \cos(h(|\mathbf{x}|))]$$

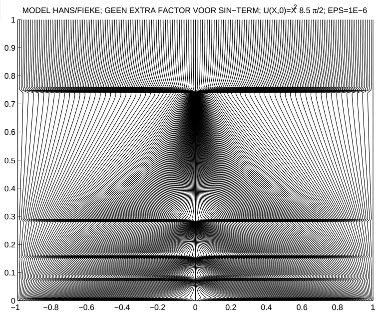
Substitution into PDE model gives (using spherical coordinates for the 2-sphere S)

$$\begin{array}{l} h_t = h_{rr} + \frac{1}{r}h_r - n^2\frac{\sin(2h)}{2r^2} \\ h(r,0) = \psi(r), \quad h(0,t) = 0, \quad h(1,t) = \psi(1) \end{array}$$

from v. Beek, 2004

Application: a model from harmonic maps [2]





Intermezzo: the heat equation

The solution of the PDE

$$\boxed{u_t = \alpha u_{xx}}$$

with

$$u(x,0) = \sin(\pi x),\;\; u(0,t) = u(1,t) = 0, \quad x \in [0,1]$$

and parameter α is given by

$$u(x,t) = e^{\alpha \pi^2 t} \sin(\pi x)$$

For $\alpha < 0$ we have *UNSTABLE* solutions, whereas for $\alpha \geq 0$ all solutions are *STABLE*.
In general, for more complicated nonlinear PDE models (with physical parameters), it is often unknown whether the solutions remain stable...

Application: the extended Fisher-Kolmogorov equation [1]

Propagation of domain walls in liquid crystals:

$$u_t + 10^{-8} u_{xxxx} = 10^{-4} \gamma u_{xx} + u - u^3, \quad x \in [0, 1]$$

(parameter γ)

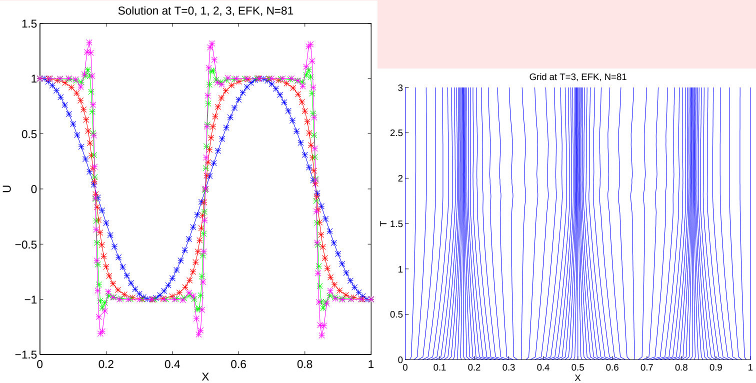
$$u(x, 0) = \cos(p\pi x)$$

$$u(0, t) = 1, \;\; u(1, t) = -1, \;\; u_x(0, t) = u_x(1, t) = 0$$

For $\gamma = -3 < \gamma_* = -\sqrt{8}$ theory predicts multi-bump solutions

from Peletier & Troy, SIAM J. Math. Anal. 1997

Application: the extended Fisher-Kolmogorov equation [2]



Application: the extended Korteweg-deVries equation [1]

Nonlinear water waves in the presence of surface tension:

$$u_t + \frac{2}{15} u_{xxxxx} + (\mu u - b) u_{xxx} + (3u + 2\mu u_{xx}) u_x = 0$$

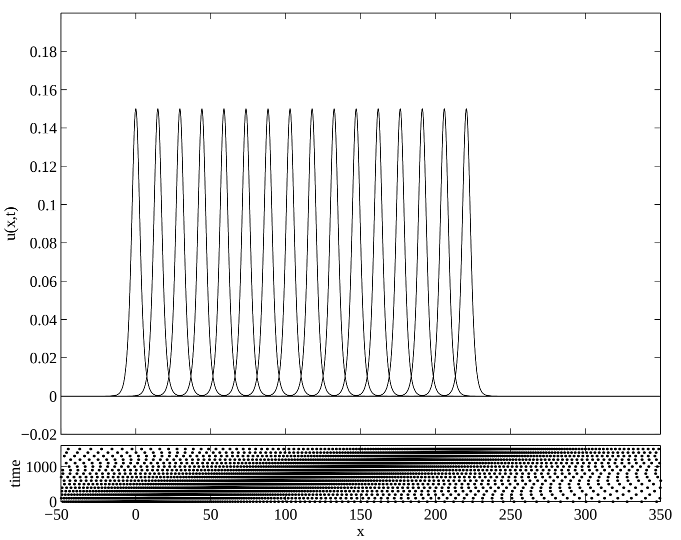
(parameter b; we set $\mu = 1$)
Explicit solutions exist:

$$u(x,t) = 3\left(b + \frac{1}{2}\right) \operatorname{sech}^2\left(\sqrt{\frac{3(2b+1)}{4}}(x + at)\right)$$

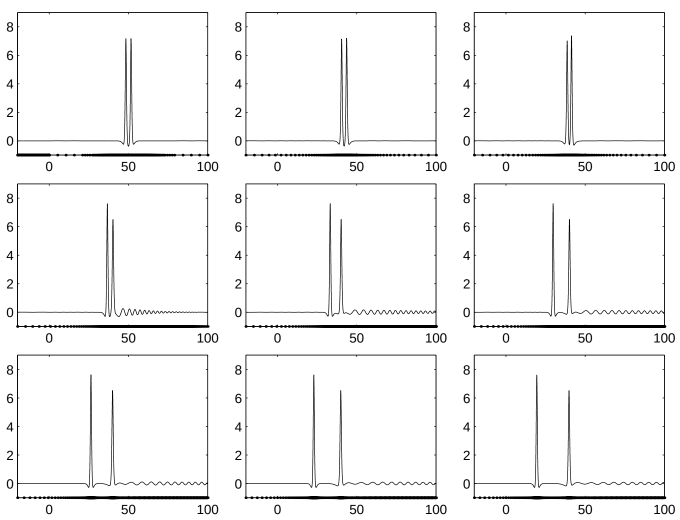
with $a = \frac{3}{5}(2b+1)(b-2),\ b \geq -1/2$. Note that $-a$ is the *velocity* of the wave.
(study stability of different types of waves for this PDE)

from P. Saucez, A. Vande Wouwer & Zegeling 2004

Application: the extended Korteweg-deVries equation [2]



Application: the extended Korteweg-deVries equation [3]



Application: the extended Korteweg-deVries equation [4]