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Multiscale Problems: Modeling, Adaptive Discretization,

Stabilization, Solvers

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High-order relaxed schemes for non linear diffusion problems

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- F. Cavalli, G. Naldi, M. Semplice in Proceedings of ENUMATH2005
- F. Cavalli, G. Puppo, G. Naldi, M. Semplice, http://arXiv.org preprint math NA/0604606, submitted SINUM

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PRIN2005

Relaxed schemes for non linear diffusion problems

Non linear (degenerate) diffusion equation

Advection-diffusion problems

Reaction-diffusion equations

$$\frac{\partial u}{\partial t} = D\Delta(p(u)), \quad x \in R^d, t > 0$$

We aim at a numerical approximation such that:

- treats non-linear p(u)
- does not exploit the form of p(u)
- treats singular p(u), as well, i.e. p(0)=0
- high order

For example, $p(u) = u^m$ (for $m > 1$) is the **porous media equation**

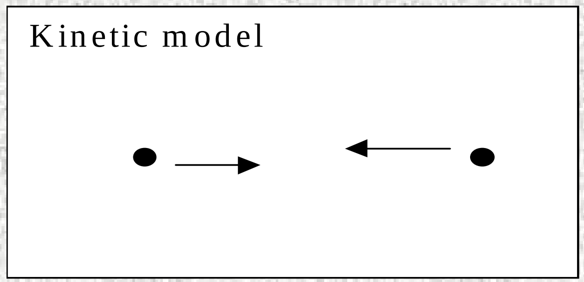
Multiscale Hyperbolic system

$$\partial_t \ldots u = \frac{1}{\varepsilon^2}(v-u)$$

Microscopic world

$$\partial_t v \ldots \frac{1}{\varepsilon}\partial_x v = \ldots \frac{1}{\varepsilon^2}(\ldots - u)$$

Goldstein-Taylor Model

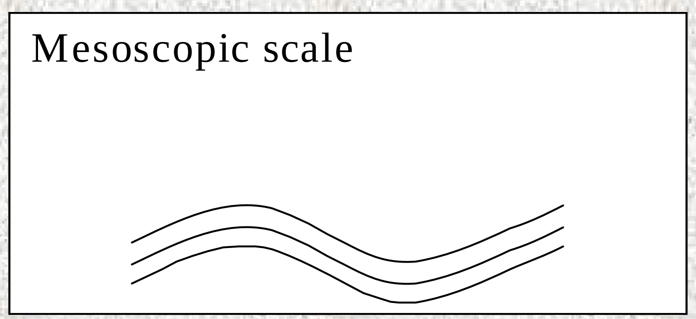


$$\begin{cases} \partial_t \rho_\varepsilon \ldots = 0 \\ \partial_t J_\varepsilon - \ldots = -\frac{2}{\varepsilon^2} J_\varepsilon \end{cases}$$

Fluid dynamical limit

$\varepsilon \rightarrow 0^+$

Maxwell-Cattaneo Model



$$\begin{cases} \partial_t \rho - \frac{1}{2} \ldots = 0 \\ J = \ldots \frac{\ldots}{2} \end{cases}$$

Diffusive limit

Linear diffusion equation, Macroscopic level

ρ = temperature , J= flux

See i.e. review work of Natalini and Marcati or the survey of S. Jin

Non linear diffusion

$$\begin{cases} \partial_t u + c\partial_x u = K(u+v,x)(v-u) \\ \partial_t v - c\partial_x v = K(u+v,x)(u-v) \end{cases}$$

diffusive scaling

$$\partial_t u + \frac{1}{\varepsilon}\partial_x u = \frac{1}{\varepsilon^2}K(u+v,x)(v-u)$$

$$\partial_t v - \frac{1}{\varepsilon}\partial_x v = \frac{1}{\varepsilon^2}K(u+v,x)(u-v)$$

Macroscopic variable

$$\begin{cases} \partial_t \rho + \partial x\, J = 0 \\ \partial_t J + \frac{1}{\varepsilon^2}\partial_x \rho = -\frac{2}{\varepsilon^2}K(\rho,x)\,J \end{cases}$$

asymptotic state

$$\partial_t \rho - \partial x\left[\frac{1}{2K(\rho,x)}\partial_x \rho\right] = 0$$

$$J = -\frac{1}{2K(\rho,x)}\partial_x \rho$$

See i.e. P.L. Lions and G. Toscani, Rev. Mat. Iberoamericana, 13:473–513, 1997

Relaxation scheme for conservation laws

Jin and Xin[1] (1995) proposed a kinetic system

$$\begin{cases} u_t + j_x = 0 \\ j_t + a u_x = -\frac{1}{\varepsilon}(j - f(u)) \end{cases}$$

to approximate the solutions of the scalar conservation laws

$$u_t + f(u)_x = 0$$

provided that $a \geq (f'(u))^2$ (*subcharacteristic condition*).
The numerical integration consists on alternation of relaxation steps

$$\begin{cases} u_t = 0 \\ j_t = -\frac{1}{\varepsilon}(j - f(u)) \end{cases} \qquad (\varepsilon \to 0) \qquad j^n = f(u(\cdot, t^n)) = f(u^n)$$

and transport steps, i.e. get $u(\cdot, t^{n+1})$ integrating on $[t^n, t^{n+1}]$

$$\begin{cases} u_t + j_x = 0 \\ j_t + a u_x = 0 \end{cases}$$

---

[1] Jin, S. and Xin, Z., The relaxation schemes for systems of conservation laws in arbitrary space dimensions *Comm. Pure Appl. Math.*, **48**(3):235-276, 1995.

Relaxation of the Laplacian operator

First introduce the auxiliary variable $v(x,t)$ and the system

$$\begin{cases} \dfrac{\partial u}{\partial t} + div(v) = 0 \\ \dfrac{\partial v}{\partial t} + \dfrac{D}{\varepsilon}\nabla p(u) = -\dfrac{1}{\varepsilon} v \end{cases}$$

Formally, in the small relaxation limit, $\varepsilon \to 0^+$, the system above approximates to leading order the nonlinear diffusion equation.

In order to have a non degenerate charcteristic velocities as $\varepsilon \to 0^+$, a suitable parameter φ is introduced and

$$\begin{cases} \dfrac{\partial u}{\partial t} + div(v) = 0 \\ \dfrac{\partial v}{\partial t} + \varphi^2 \nabla p(u) = -\dfrac{1}{\varepsilon} v + \left(\varphi^2 - \dfrac{D}{\varepsilon}\right)\nabla p(u) \end{cases}$$

Relaxation of the non-linearity

So far we turned the (degenerate) nonilnear diffusion operator into a nonlinear hyperbolic system with stiff source terms

We now introduce another variable *w* and rewrite the system above as

$$\begin{cases} \dfrac{\partial u}{\partial t} + div(v) = 0 \\ \dfrac{\partial v}{\partial t} + \varphi^2 \nabla w = -\dfrac{1}{\varepsilon} v + \left(\varphi^2 - \dfrac{D}{\varepsilon} \right) \nabla w \\ \dfrac{\partial w}{\partial t} + div(v) = -\dfrac{1}{\varepsilon} \left(w - p(u) \right) \end{cases}$$

This is now a semilinear hyperbolic system with stiff source terms of the kind usually exploited in relaxation schemes.

Relaxed schemes for non linear diffusion problems

Advantages of the method

• the (degenerate) non-linear problem becomes (non degenerate) semi-linear

•fronts and discontinuities should be tracked faithfully by methods designed for hyperbolic equations

•no need for nonlinear solvers nor Riemann solvers

• very simple to generalize for different $p(u)$

• easy implementation on parallel computer

A first/second order scheme had been already studied by Naldi, Pareschi (SINUM 2000) and Naldi, Pareschi, Toscani (Surv. Ind. Math., 2002)

Preliminary work on high order schemes for this relaxation system in Proceedings ENUMATH2005.

Relaxed schemes for non linear diffusion problems

Outline

We studied and implemented the relaxed schemes obtained by choosing $\varepsilon = 0$ in the above relaxation system with:

- high order spatial reconstructions (ENO/WENO)
- appropriate time integrators (IMEX of matching accuracy)

♦ semidiscrete scheme
♦ proof of convergence
♦ nonlinear stability for the low order scheme
♦ linear stability for the higher order schemes
♦ numerical accuracy and convergence tests

Relaxed schemes for non linear diffusion problems

Semidiscrete relaxed IMEX Runge-Kutta scheme

The relaxation system may be cast in the form z_t +div $f(z)$ = g(z)/ε and we integrate in time as (with uniform time step Δt)

$$z^{n+1} = z^n - \Delta t \sum_{i=1}^{m} \tilde{b}_i \frac{\partial f}{\partial x}(z^{(i)}) + \frac{\Delta t}{\varepsilon} \sum_{i=1}^{m} b_i \; g(z^{(i)})$$

where

$$z^{(i)} = z^n - \Delta t \sum_{k=1}^{i-1} \tilde{a}_{i,k} \frac{\partial f}{\partial x}(z^{(k)}) + \frac{\Delta t}{\varepsilon} \sum_{k=1}^{i} a_{i,k} \; g(z^{(k)})$$

Here $(\tilde{a}_{i,k}, \tilde{b}_i)$ and (a_{ik}, b_i) are a pair of Butcher's tableaux (for nonzero ε we need IMEX SSP).

Relaxed schemes for non linear diffusion problems

Semidiscrete relaxed IMEX Runge-Kutta scheme (II)

For $i = 1$, we let $\varepsilon \to 0$ in (now Φ^2 is a diagonal matrix times φ^2)

$$\begin{bmatrix} u^{(1)} \\ v^{(1)} \\ w^{(1)} \end{bmatrix} = \begin{bmatrix} u^{n} \\ v^{n} \\ w^{n} \end{bmatrix} + \frac{\Delta t}{\varepsilon} a_{1,1} g\left(\begin{bmatrix} u^{(1)} \\ v^{(1)} \\ w^{(1)} \end{bmatrix} \right) = \begin{bmatrix} u^{n} \\ v^{n} \\ w^{n} \end{bmatrix} + \frac{\Delta t}{\varepsilon} a_{1,1} \begin{bmatrix} 0 \\ -v^{(1)} + (\varepsilon\Phi^2 - D) w_x^{(1)} \\ -w^{(1)} + p(u^{(1)}) \end{bmatrix}$$

and therefore

$$u^{(1)} = u^n \qquad w^{(1)} = p(u^{(1)}) \qquad v^{(1)} = -D w_x^{(1)}.$$

Relaxed schemes for non linear diffusion problems

Semidiscrete relaxed IMEX Runge-Kutta scheme (III)

For i =2,

$$z^{(2)} = z^n - \Delta t \tilde{a}_{2,1} f(z^{(1)}) + \frac{\Delta t}{\varepsilon} a_{2,1} \underbrace{g(z^{(1)})}_{=0} + \frac{\Delta t}{\varepsilon} a_{2,2} g(z^{(2)})$$

$$\Longrightarrow \quad \begin{cases} u^{(2)} = u^n - \Delta t \tilde{a}_{2,1} v_x^{(1)} \\ w^{(2)} = p(u^{(2)}) \\ v^{(2)} = -D w_x^{(2)} \end{cases}$$

Summarizing, the relaxed scheme reduces to an alternation of relaxation steps and transport steps.

Relaxed schemes for non linear diffusion problems

Semidiscrete relaxed IMEX Runge-Kutta scheme (IV)

relaxation steps

$$g(z^{(i)}) = 0 \qquad \text{i.e.} \quad \begin{cases} w^{(i)} = p(u^{(i)}) \\ v^{(i)} = -\nabla w^{(i)} \end{cases}$$

transport steps (we advance for time $\tilde{a}_{i,k}\,\Delta t$)

$$z_t + \operatorname{div} f(z) = 0$$

with initial data $z = z^{(i)}$, retain only the first component and assign it to $u^{(i+1)}$.

Finally the value of u^{n+1} is computed as $u^n + \sum \tilde{b}_i\, u^{(i)}$.

Relaxed schemes for non linear diffusion problems

Convergence theorem

Let $u(x, t)$ be the weak solution of
$$\begin{cases} \frac{\partial u}{\partial t} = D\Delta(p(u)), \quad x \in R^d, t > 0 \\ u(x,0) = u^0(x) \end{cases}$$

$u^n(\cdot,t)$ be the semidiscrete approximate solution obtained for time t as described. Assume $u^0 \in L^\infty, \|u^0\|_\infty = M$ and that p be a non-decreasing Lipschitz continuous on [-M,M]. If the following conditions hold

$$\begin{cases} \alpha_{ik} \geq 0, \beta_{ik} \geq 0, \\ \alpha_{ik} = 0 \Rightarrow \beta_{ik} = 0, \\ \sum_{k=1}^{i-1} \alpha_{ik} = 1 \text{ (consistency)}, \\ \frac{\mu\tau}{\sigma\tau} \leq \min_{\alpha_{ik} \neq 0} \frac{\alpha_{ik}}{\beta_{ik}} \quad \text{(stability)}, \end{cases}$$

then $\lim_{n\to\infty} u^{(n)} = u(t)$ in L^1. Moreover the convergence is uniform for t in any given bounded interval.

Relaxed schemes for non linear diffusion problems

relaxed IMEX scheme: implicit part

Introduce a regular grid with $x_j = a - h/2 + jh$ at the centre of the computational cells, for $j = 1,\ldots,N$ and $h = (b-a)/N$. Let $u_j = u(x_j)$,
The implicit part of the scheme, in the relaxed version simplyfies to the resolution of a triangular system, which may be obtained using only function evaluations.

$$w^{(i)} = p(u^{(i)}) \qquad v^{(i)} = -D\widehat{\nabla_x} w^{(i)}$$

For second order, we use simply the Heun method and for third order the scheme with the followin tableaux

$$\begin{array}{c|ccc} & 0 & 0 & 0 \\ & 1 & 0 & 0 \\ & \frac{1}{4} & \frac{1}{4} & 0 \\ \hline & \frac{1}{6} & \frac{1}{6} & \frac{2}{3} \end{array}$$

Relaxed schemes for non linear diffusion problems

relaxed IMEX scheme: explicit part

The transport steps, may be thougth as the time advancement of the first component of the system

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \\ w \end{pmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & \Phi^2 \\ 0 & 1 & 0 \end{bmatrix} \frac{\partial}{\partial x}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = 0$$

The characteristic variables that diagonalize the system are

$$U = \tfrac{v+w}{2} \quad V = \tfrac{w-v}{2} \quad W = u - w \qquad \text{and } u = U + V$$

$$\text{speed}=\Phi \quad \text{speed}=-\Phi \quad \text{speed}=0$$

$$\Longrightarrow \begin{array}{l} u_j^{(i)} = u_j^n - \Delta t \sum_{k=1}^{i-1} \tilde{a}_{i,k}\left[\Phi\left(U_{j+1/2}^{(i)-} - U_{j-1/2}^{(i)-}\right) - \Phi\left(V_{j+1/2}^{(i)+} - V_{j-1/2}^{(i)+}\right)\right] \\ u_j^{n+1} = u_j^n - \lambda \sum_{i=1}^{\nu} \tilde{b}_i\left[\left(U_{j+1/2}^{(i)-} - V_{j+1/2}^{(i)+}\right) - \left(U_{j-1/2}^{(i)-} - V_{j-1/2}^{(i)+}\right)\right] \end{array}$$

Where $U_{j\pm1/2}^{(i)\pm}$ and $V_{j\pm1/2}^{(i)\pm}$ are suitable non-oscillatory reconstructions (limiters, ENO, WENO).

Relaxed schemes for non linear diffusion problems

Non-linear stability

We performed non-linear stability analysis on the first order scheme for
$u_t - \Delta(p(u))=0$ (piecewise constant reconstructions and Euler timestepping)

$$u_j^{n+1} = u_j^n - \frac{\lambda}{2}\left(\partial_x p(u^n)|_{j+1} - \partial_x p(u^n)|_{j-1}\right) + \frac{\lambda}{2}\Phi\left(p(u_{j+1}^n) - 2p(u_j^n) + p(u_{j-1}^n)\right)$$

One may prove that (when using central differences to approximate $\partial_x p(u)$)

$$\mathrm{TV}(u^{n+1}) \le \mathrm{TV}(u^n)$$

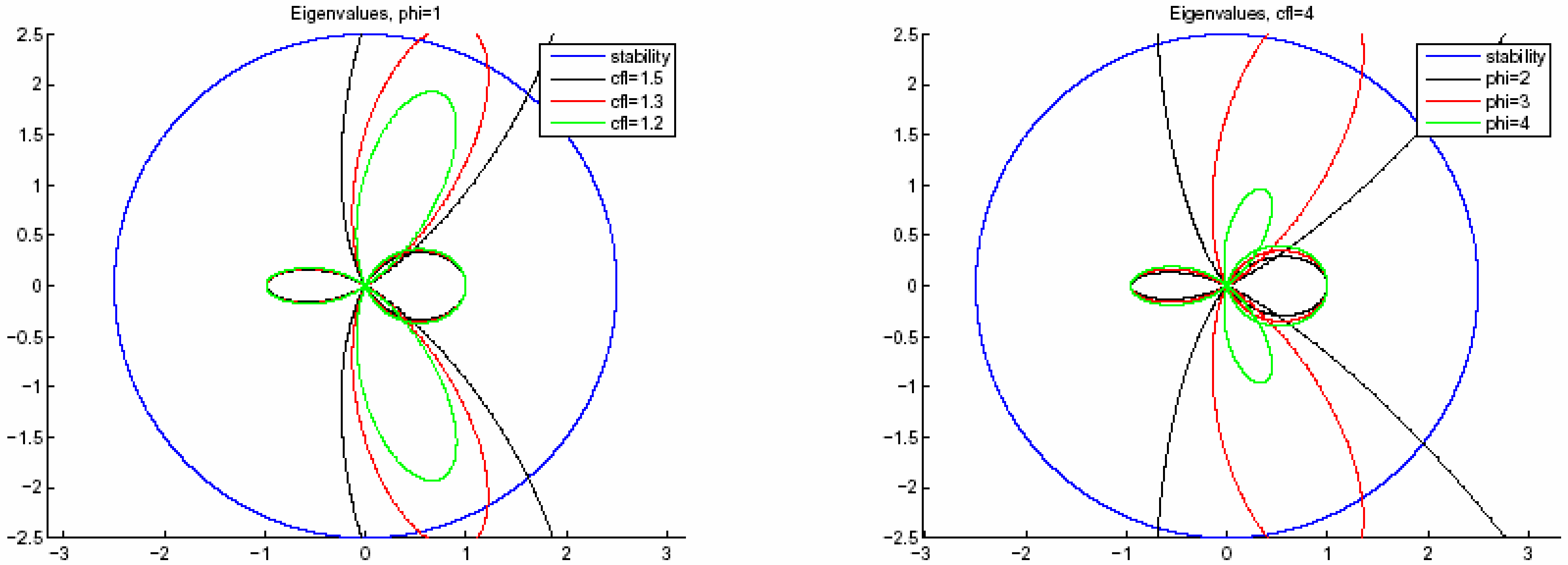
provided that $\Delta t \le 2h^2/\mu$, where μ is the Lipshitz constant of the function p.

(Using upwind/downwind approximations for ∂x in order to reduce the stencil gives much stronger stability constraints)

Relaxed schemes for non linear diffusion problems

Linear stability

Regarding the higher order schemes, we performed a linear stability analysis, setting $p(u)=u$ and computing the amplification factors of each Fourier mode in a VonNeumann analysis. Varying Φ and the constant C such that $\Delta t = C h^2$ we obtain:



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Relaxed schemes for non linear diffusion problems

Non periodic boundary conditions

Dirichlet or Neumann boundary conditions in 1D may be easily implemented with the following procedure:

- add extra points to the computational grid outside the domain Ω;
- (e.g. at the left boundary $x = 0$ of the domain Ω) choose a polynomial $p^{(k)}(x)$ of degree k that fits the points u_1^n, u_2^n,…, u_k^n and that satisfies the given b.c. on the border $x = 0$;
- use the polynomial $p(k)(x)$ to set the values of the points u_0^n, u_{-1}^n,…;
- apply the algorithm in Ω. The values of u_0^n, u_{-1}^n,... will be used in the calculations.

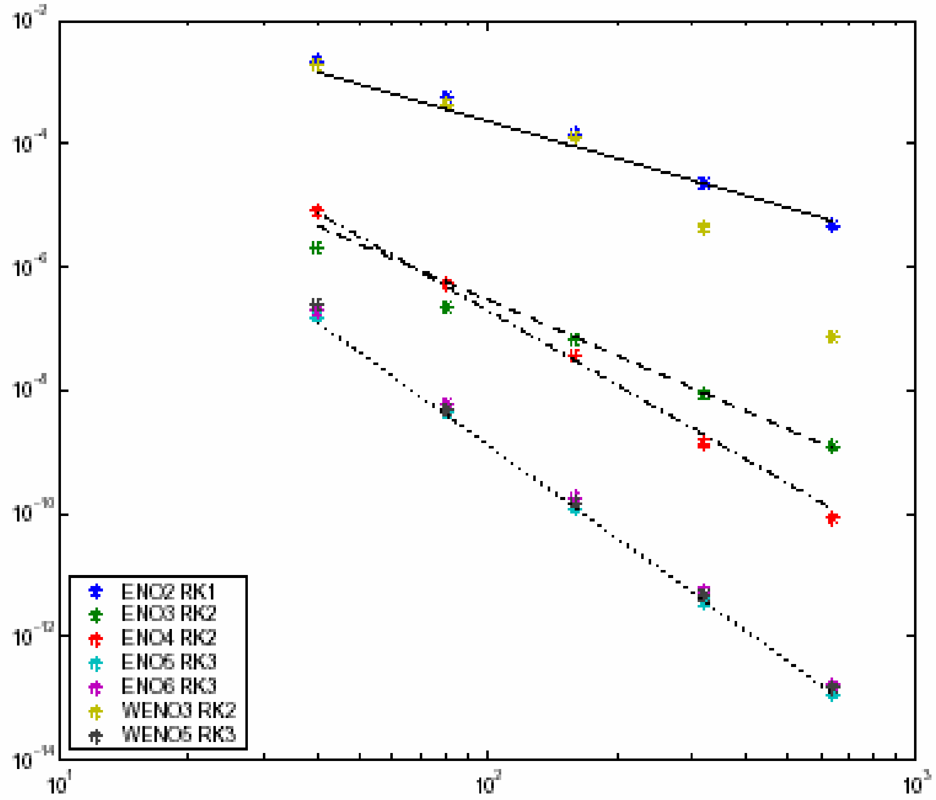
The number of points to add depends on the degree of the scheme and on the implementation, but only the given boundary condition for $u(x)$ is used to set the values.

Relaxed schemes for non linear diffusion problems

1D results (1): linear equation with Neumann b.c.

Linear diffusion equation

$$\begin{cases} u_t = u_{xx} \text{ on } [0,1] \\ u_0(x) = x + \cos(2\pi x) \\ u_x|_{x=0,1} = 1 \end{cases}$$



(The reduced rate of the ENO6/RK3 scheme is due to the implementation of the boundary conditions)

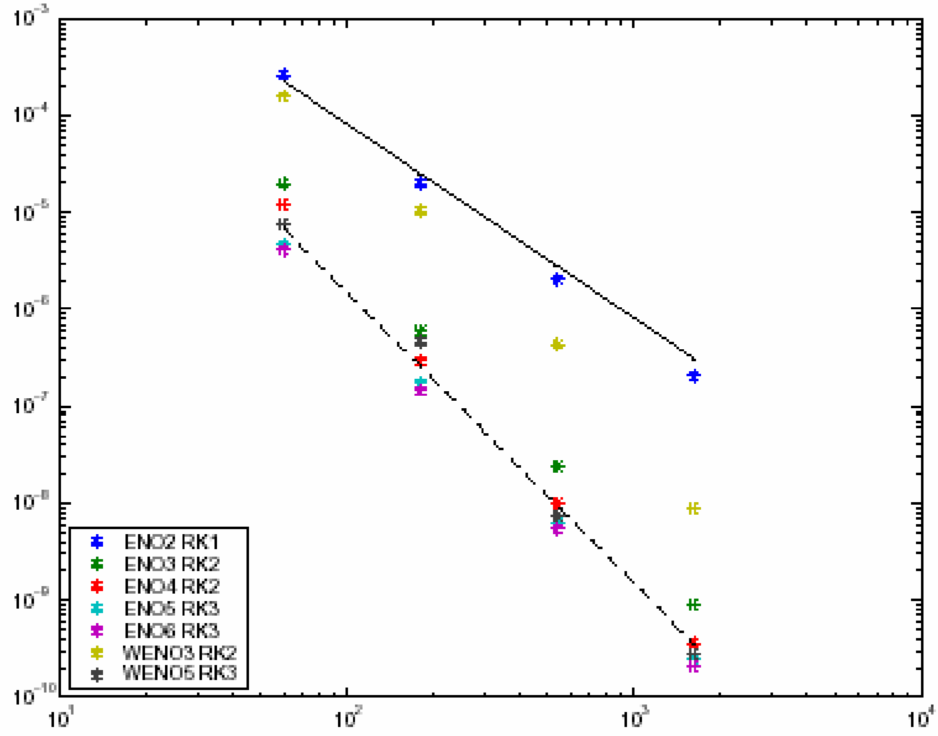
Relaxed schemes for non linear diffusion problems

1D results (2): $u_t + \Delta u^2 = 0$

We took initial data of class C^1 with compact support and set the final time of integration such that no front had developed yet.

With smoother initial data one recovers the higher convergence rates.

Even after the front develops (u_x becomes discontinuous in finite time), the higher order schemes provide reduced errors.



Relaxed schemes for non linear diffusion problems

$$\Omega \subseteq \mathrm{R}^d$$

One may obtain schemes for regular grids in R^d by addittive dimensional splittin
Let $u^n{}_J$ be the values of $u(x_J, t^n)$, where $J=(j_1, j_{2,\ldots,} j_d)$ is a multi-index of d integers. The relaxation steps are straightforward.
For each Euler step of the transport equation, consider the collection of 1D problems for $u^n(\ldots, jm\text{-}1, \bullet, jm+1, \ldots)$ where only the m[th] spatial variable is left and all the others are fixed. Save the corresponding increment

$$\Delta^n_{(m),J} = \left[\Phi\left(U^-_{jm+1/2} - U^-_{jm-1/2}\right) - \Phi\left(V^+_{jm+1/2} - V^+_{jm-1/2}\right)\right]$$

Then update

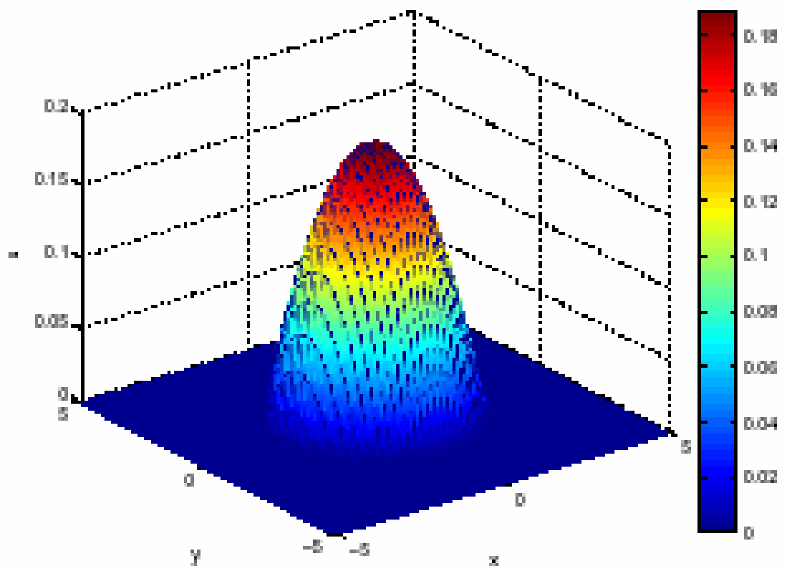
$$u^{n+1}_J = u^n_J + \sum_{m=1}^{d} \Delta^n_{(m),J}$$

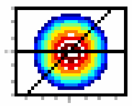
Applying this procedure for each stage value of the Ringe-Kutta scheme, we are able to generalize our schemes to $\mathbb{R}^d$

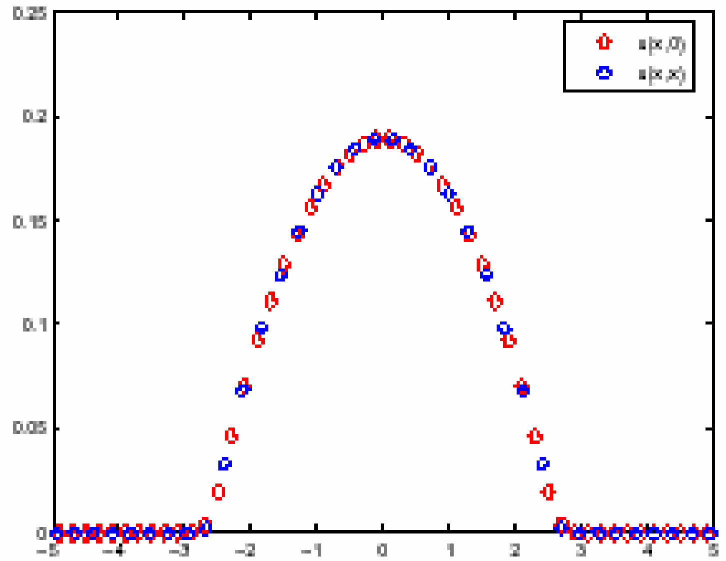
Relaxed schemes for non linear diffusion problems

2D results: simmetry

We tested that the scheme of second order for $u_t + \Delta u^2 = 0$, with the Barenblatt initial data maintain the spherical symmetry in time. Below is a superposition of two cross-sections along $x = 0$ and $y = x$.

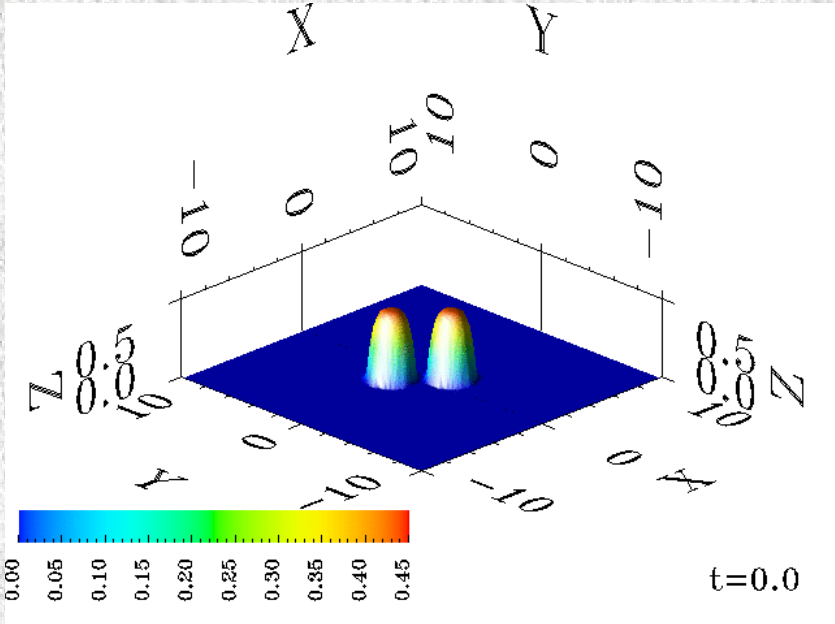


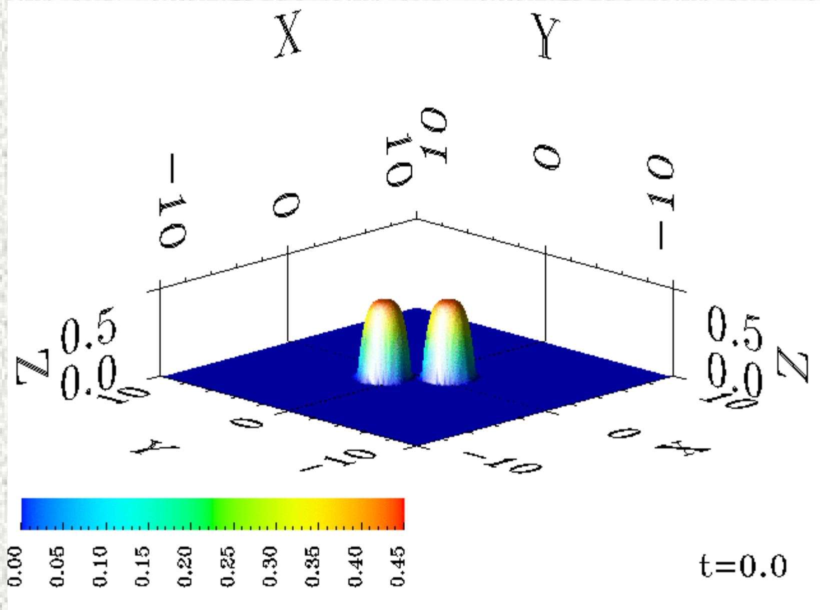




Relaxed schemes for non linear diffusion problems

2D results: two bumps

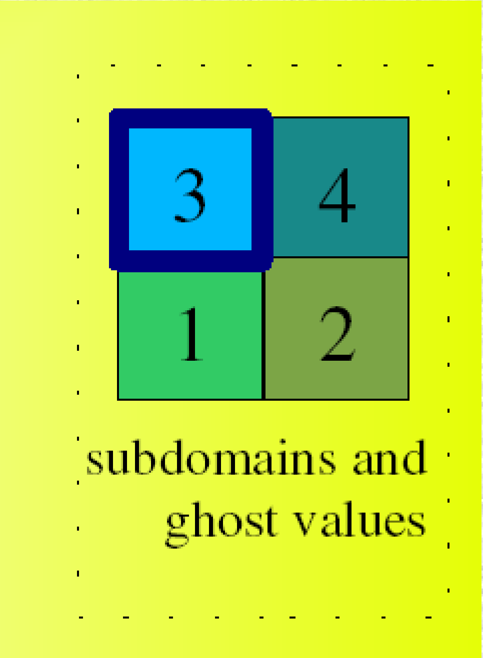




Parallel Algorithms (I)

Implementation on a cluster of parallel processors (thanks to www.petsc.org and the IT staff of the Department of Mathematics - Milano)

The problem is broken into subproblems solved by distinct processors, that exchange information on the boundary nodes at each integration step. This is needed in the ENO reconstruction procedure that has a stencil (k-1) nodes wide and for boundary conditions.

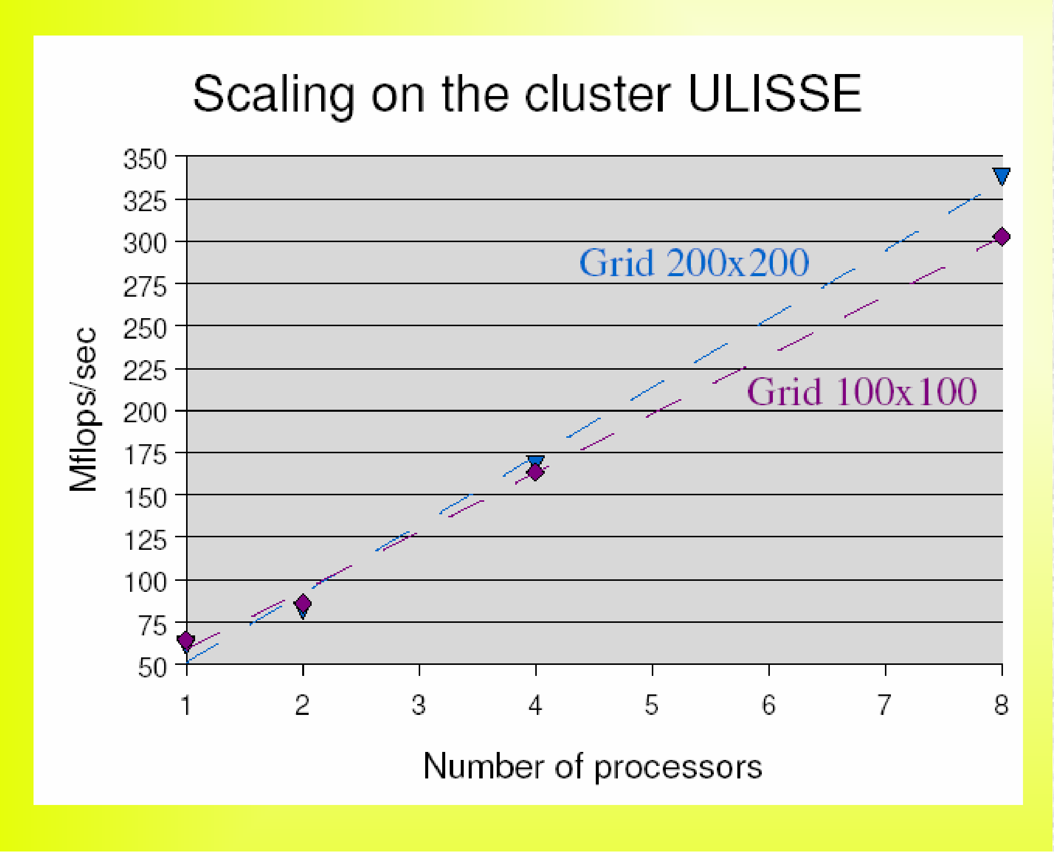


Our code:

- exploits PETSC libraries and parallel linpack/lapack libraries
- our ENO library: can reconstruct in any degree k. It uses only MatVec multiplies, so scales essentially linearly with the number of processors.
- We implemented schemes of order 2,3,5,6 for 1D and 2D

Parallel Algorithms (II)

The algorithm shows a good (linear!) scaling behaviour, until the subproblems assigned to each processor become too small and the time spent exchanging MPI messages among the processors become predominant (the overhead of MPI communications among processors shows up as reduced speedup on the smaller grid).



Conclusions

- relaxation removes the degeneracy of the differential operator
- relaxation moves the non-linearity from the differential operator and into the source terms
- we use high order schemes for hyperbolic equations

the schemes involve only function evaluations and matrix-vector products; for the relaxed schemes, no need to solve linear or nonlinear systems.

- easy extension to more space dimensions
- easy to implement on parallel computers
- convergence proof
- linear stability for high order schemes, nonlinear stability for the first order scheme
    - upcoming more general stability results
    - $\varepsilon \neq 0$
    - possible extensions to convection-diffusion equations

More complex problem **Advection-diffusion problem**

A more complex application ...

Collaboration with A. Gamba (Politecnico Torino), D. Valdembri and G. Serini (Institute for Cancer Research and Treatment, Candiolo)

Vascular Networks form by the spontaneous aggregation of endothelial cells migrating toward vascularization sites.
We have the following essential steps in the early stage of the phenomena:

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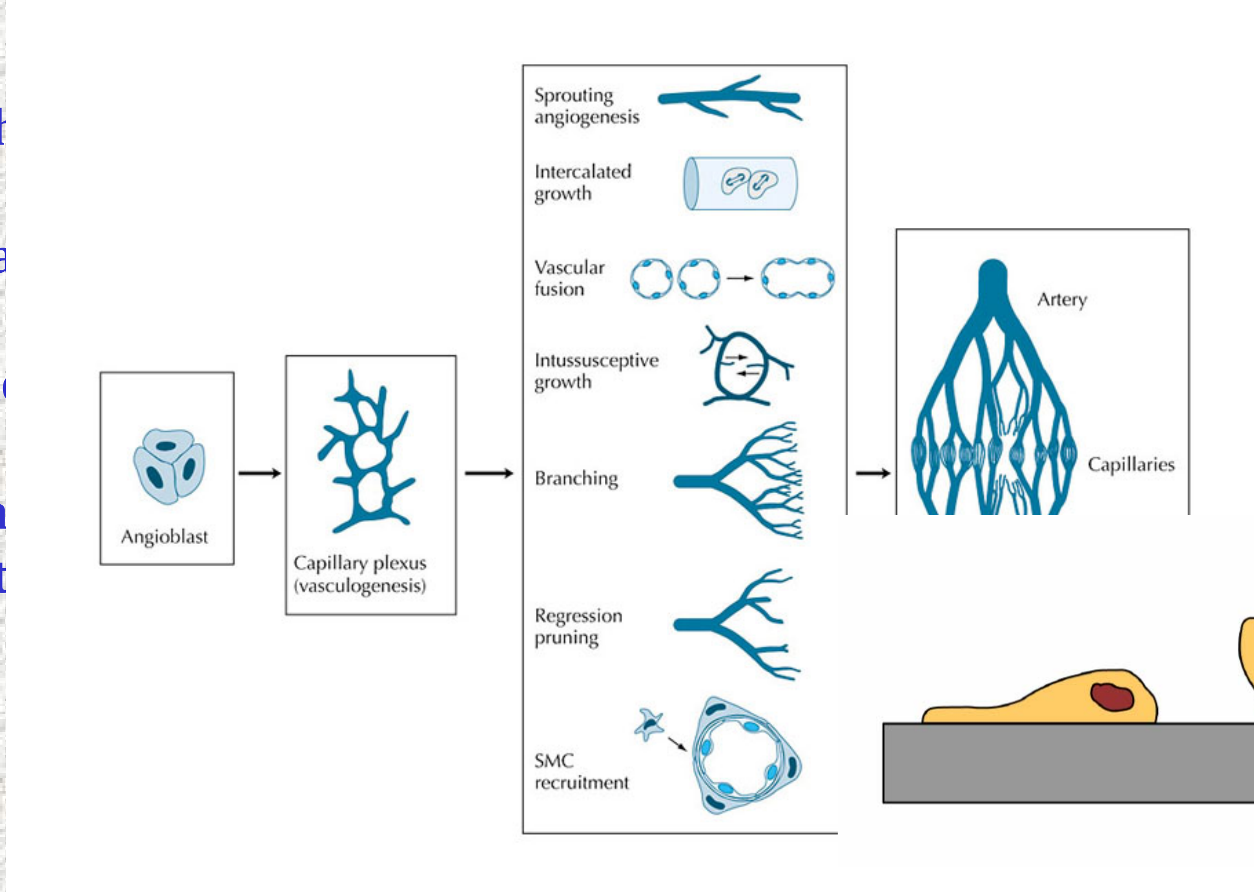
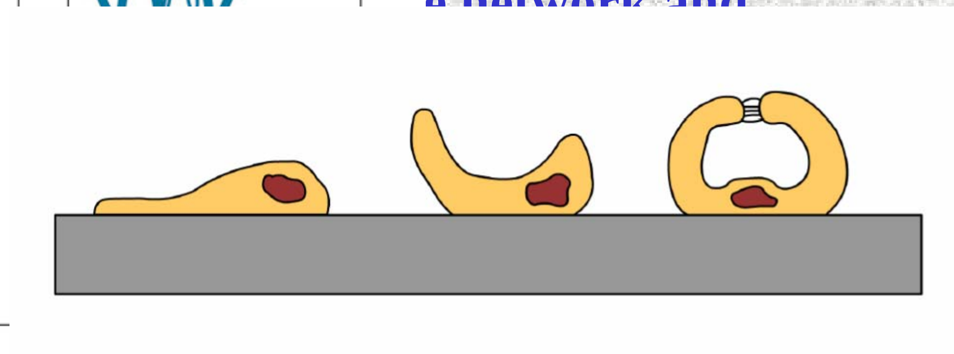
•angiobla

•elongati

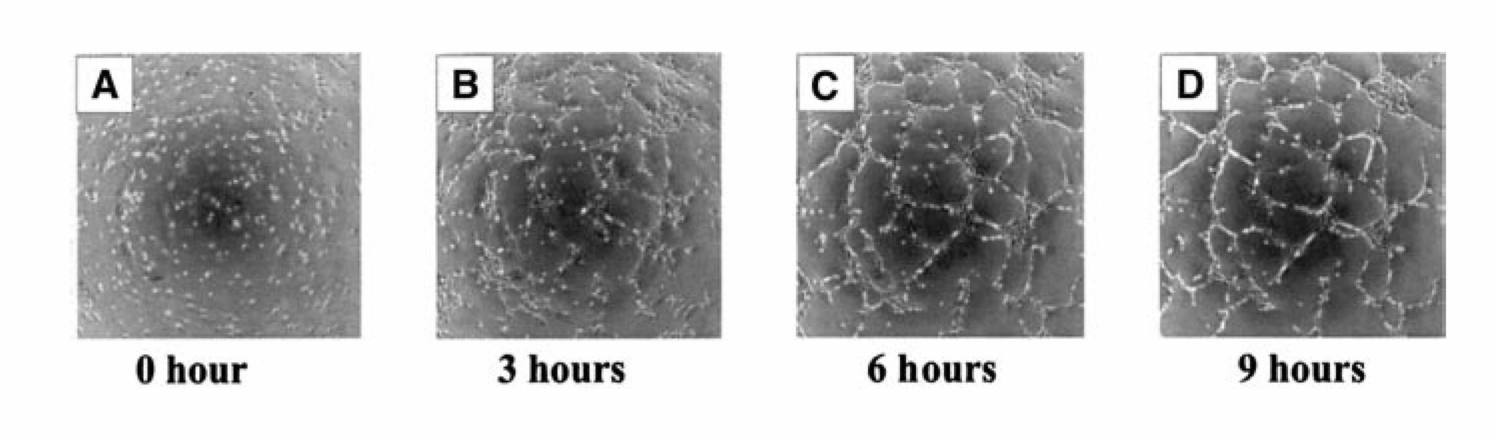
•the orga ... e network and concomit





Starting point: EXPERIMENTAL OBSERVATIONS in 2D

in vitro vascularization experiments.

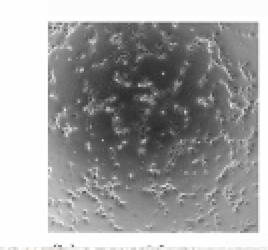
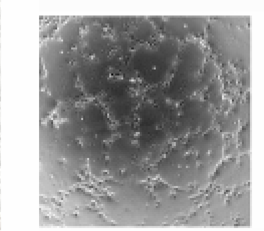


From G. Serini et al.
The EMBO Journal Vol. 22 No. 8
pp. 1771-1779, 2003

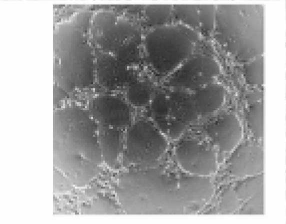
Capillary patterns are closely mimicked by endothelial cells cultured on Matrigel, a preparation of basement membrane proteins. On the Matrigel surface, single randomly dispersed endothelial cells self-organize into vascular networks.

The process of formation of a vascular-type network follows three main steps:

(i) endothelial cells migrate independently, adhere with closest neighbours, and eventually form a continuous multicellular network.

(ii) In the second step the network just undergoes a slow deformation;

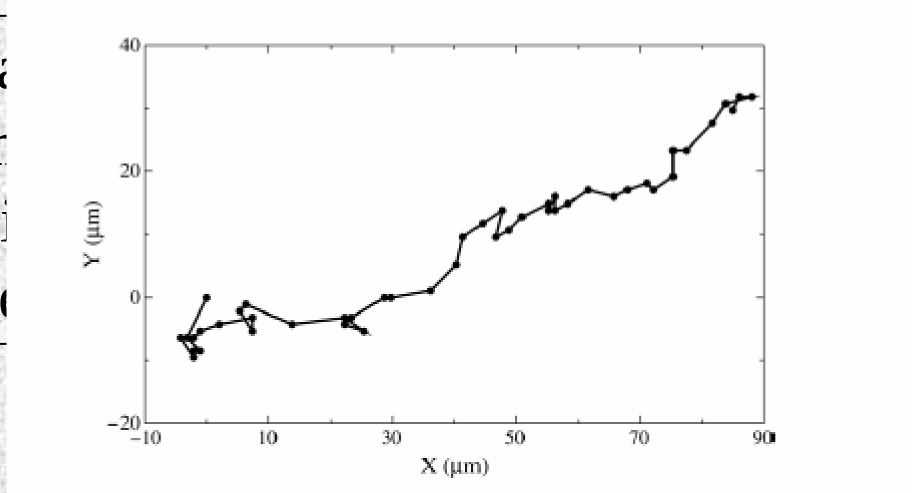


(iii) Finally, individual cells fold up to form capillary-like tubes.

Total time: 12/15 h

Observation of cell trajectories

Tracking of individua | e in the direction of
cell motion, with a sm | sed
(Serini *et al.*, 2003): i | tly directed toward
zones of higher conce



This suggests that a mechanism of cell crosstalk is present in the system. Recent works (Carmeliet, 2000; Helmlinger *et al.*, 2000) confirm that endothelial cells in the process of vascular network formation exchange signals by the release and absorption of VEGF-A.

This growth factor can bind to specific receptors on the cell surface and induce motion along its concentration gradients (chemotaxis phenomena)

It is possible to describe cellular matter by means of a continuous density field n(x,t) and the corresponding velocity field **v**(x,t)

The cells are triggered by chemical gradients due to the presence of a chemical concentration field c(x,t) (chemoattractant created by the cells themselves).

$$x \in \Omega = [0, L]^d \subset R^d, d = 2,3$$

$$t \geq 0,$$

periodic boundary conditions

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \\ \dfrac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = \mu(c) \nabla c - \nabla p(n) - \beta(c)\mathbf{v} \\ \dfrac{\partial c}{\partial t} = D\Delta c + \alpha(c) f(n) - \dfrac{c}{\tau} \end{cases}$$

(Gamba et al., PRL, 90, 2003)

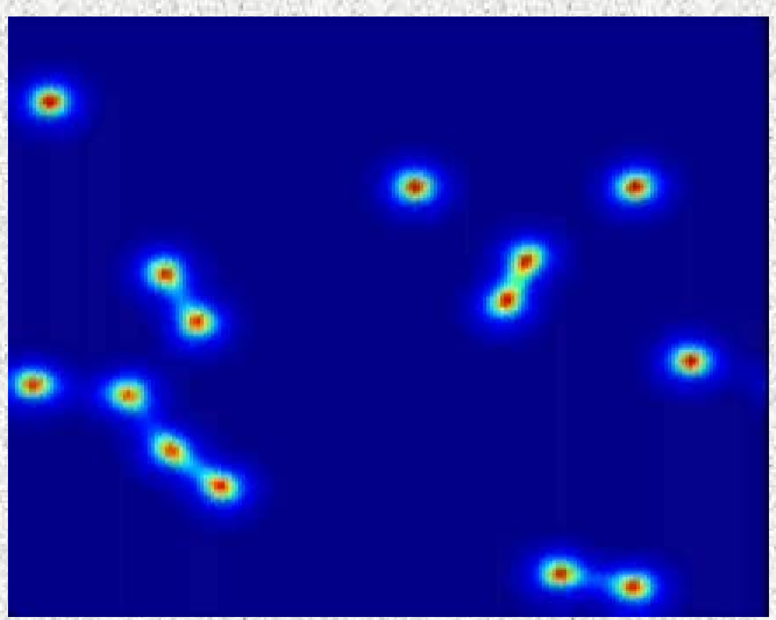
Mass conservation and cells motion

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{v}) = 0$$

Conservation law

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = \ldots\ldots\ldots$$

Multidimensional Burger's equation (Amoeboid cell movements)



Forces

$\beta \approx 10^{-3} s^{-1}$

Pressure

Friction

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = \mu(c)\nabla c - \nabla p(n) - \beta(c)\mathbf{v}$$

Chemotactic force

Diffusion of chemoctactic factor

Diffusion

$$\frac{\partial c}{\partial t} = D\Delta c + \alpha(c)\,n - \frac{c}{\tau}$$

$D_c \approx 10^{-5} mm^2 / s$

$D_r \approx \sigma^2 / \tau \approx 10^{-8}$

degradation

$\tau \approx 4000s$

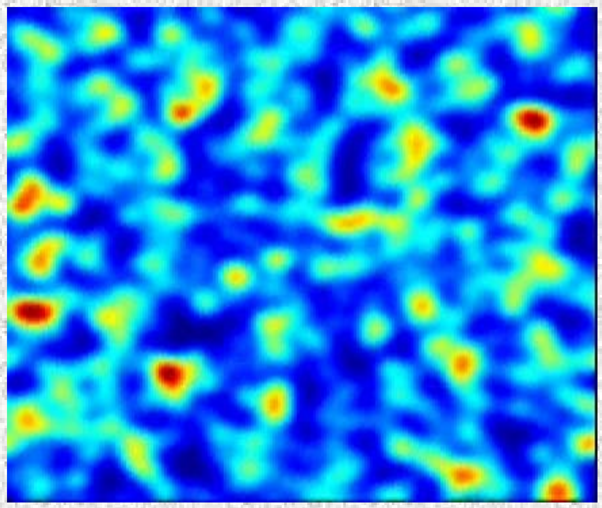
source

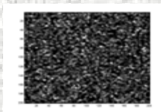
$\alpha_c = 0.4$

$\alpha_r = 0.001$

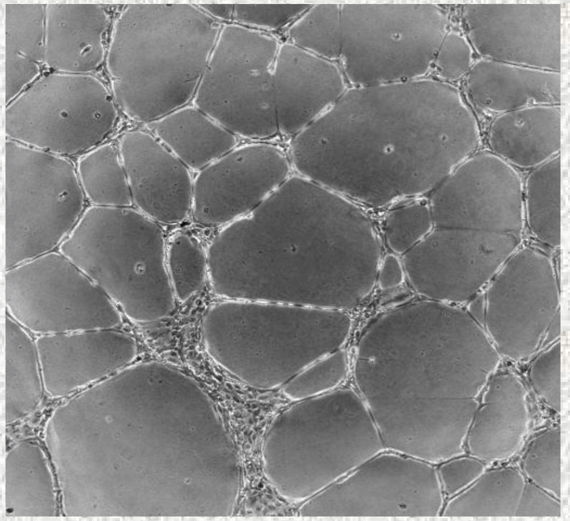
2D SIMULATIONS

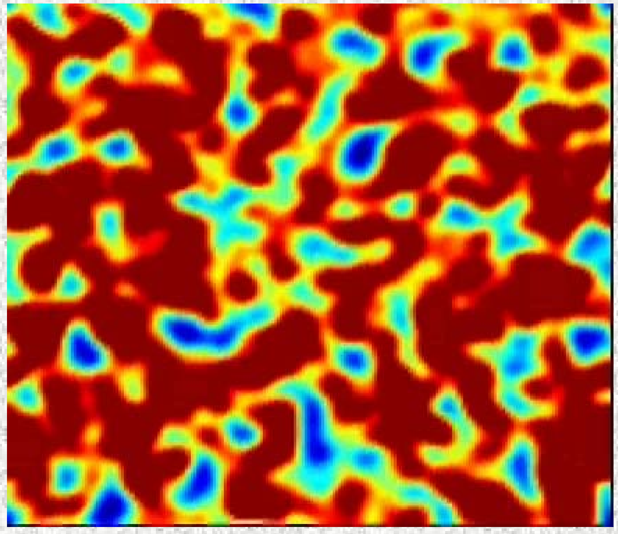
Experiments from IRCC

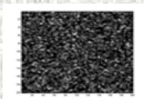




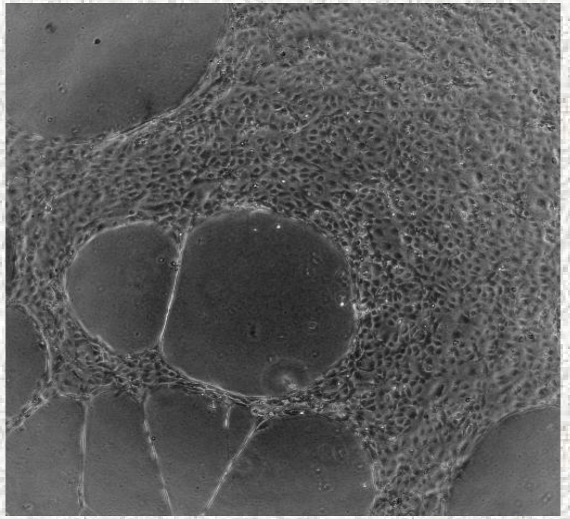
200 $cell / mm^2$





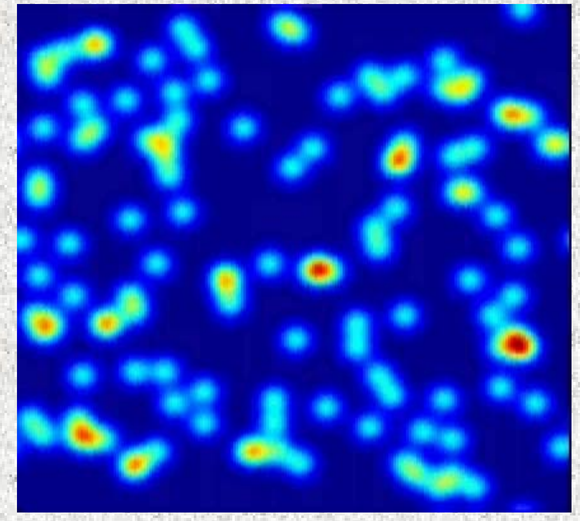


400 $cell / mm^2$

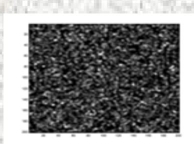


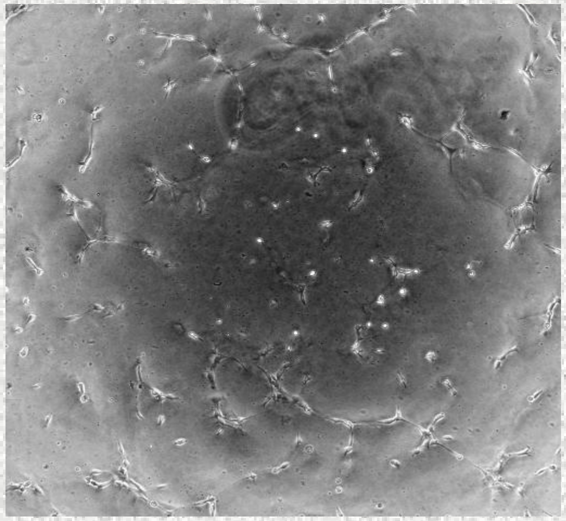
2D SIMULATIONS

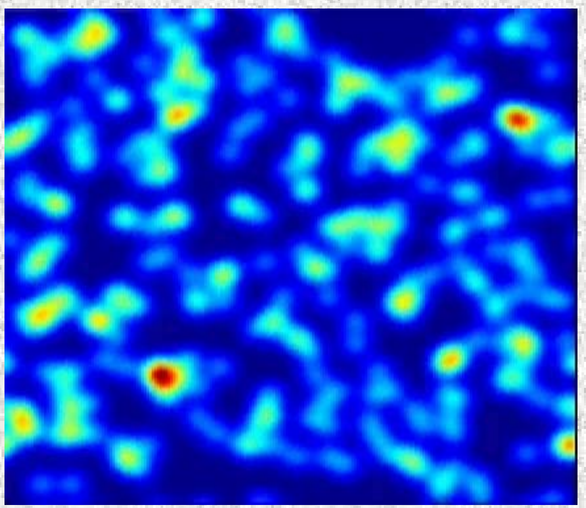
Experiments from IRCC



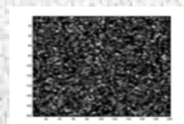
$50\ cell\ /\ mm^2$

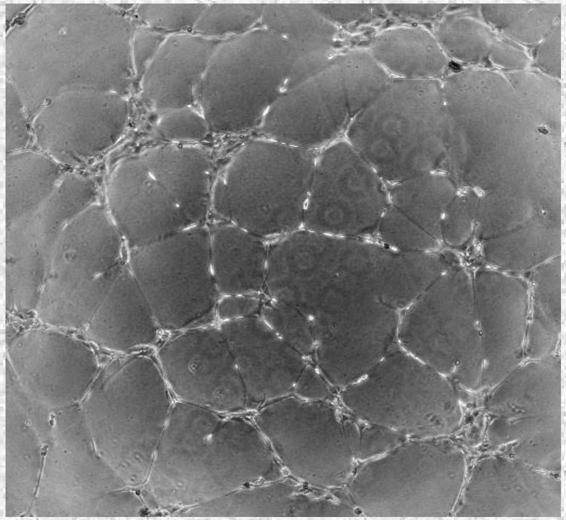






$100\ cell\ /\ mm^2$





3D SIMULATIONS

Experimental data

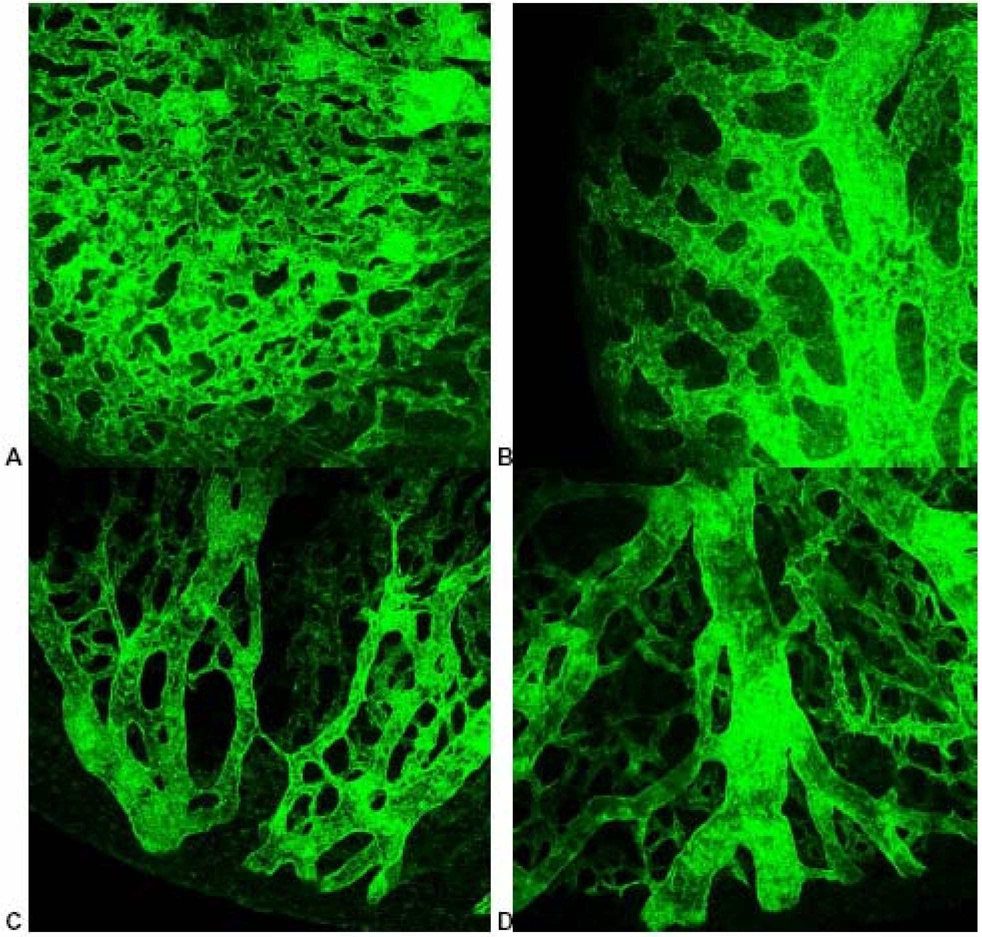
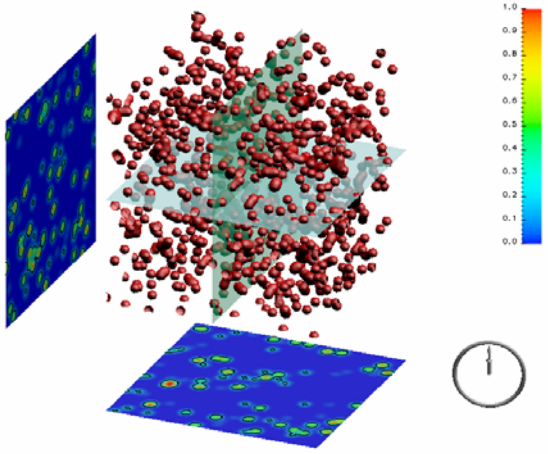
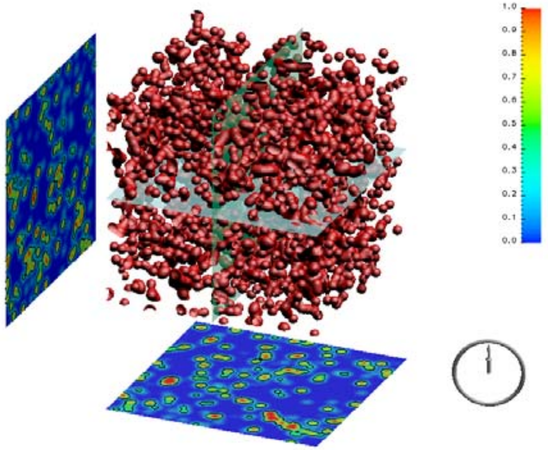


Fig. 1. Vascular networks formed by vasculogenesis in chick embryo brain, at variuos stages of development, classified according to Hamilton and Hamburger (HH). **A**: HH stage 17; **B**: HH stage 20; **C**: HH stage 26; **D**: HH stage 26.





Problem

Convection diffusion equation

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \frac{\partial^2 p(u)}{\partial x^2}, \qquad x \in \mathbb{R}, \quad t > 0$$

We want that our numerical approximation

- treats *non-linear* $p(u)$ (Lipshitz continuous, non decreasing) and *non-linear* $f(u)$ (Lipshitz continuous)
- treats the degenerate parabolic regime $p(u) = 0$ as well as the purely diffusive one, i.e. $f(u) = 0$
- *high order* in space and time
- does not exploit the form of the non linearities $p(u), f(u)$

Relaxation scheme for the convection diffusion equation

Starting equations

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \frac{\partial^2 p(u)}{\partial x^2}, \qquad x \in \mathbb{R}, \quad t > 0$$

Relaxation of the *diffusion* term

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial v}{\partial x} + \dfrac{\partial f(u)}{\partial x} = 0 \\ \dfrac{\partial v}{\partial t} + \Phi^2 \dfrac{\partial w}{\partial x} = -\dfrac{1}{\varepsilon} v + \left(\Phi^2 - \dfrac{1}{\varepsilon} \right) \dfrac{\partial v}{\partial x} \\ \dfrac{\partial w}{\partial t} + \dfrac{\partial v}{\partial x} = -\dfrac{1}{\varepsilon}(w - p(u)) \end{cases}$$

We have to introduce another auxiliary variable z to relax the convection term: we have two choiches

- $z = f(u)$
- $z = v + f(u)$

Relaxation scheme for the convection diffusion equation

We choose $z = v + f(u)$, gaining

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial z}{\partial x} = 0 \\ \dfrac{\partial v}{\partial t} + \Phi^2 \dfrac{\partial w}{\partial x} = -\dfrac{1}{\varepsilon} v + \left(\Phi^2 - \dfrac{1}{\varepsilon} \right) \dfrac{\partial v}{\partial x} \\ \dfrac{\partial w}{\partial t} + \dfrac{\partial v}{\partial x} = -\dfrac{1}{\varepsilon}(w - p(u)) \\ \dfrac{\partial z}{\partial t} + A^2 \dfrac{\partial u}{\partial x} = -\dfrac{1}{\varepsilon}(z - v - f(u)) \end{cases}$$

Advantages of $z = v + f(u)$ versus $z = f(u)$:

- A less diffusive numerical scheme
- Full freedom in picking Φ
- Only two characteristic variables to reconstruct as $z = U + V$

Semidiscrete relaxed IMEX Runge-Kutta scheme

The relaxation system can be cast in the form

$$s_t + \frac{\partial g(s)}{\partial x} = \frac{1}{\epsilon} h(s)$$

Time integration

$$\begin{cases} s^{(i)} & = s^n - \Delta t \sum_{k=1}^{i-1} \tilde{a}_{i,k} \dfrac{\partial g}{\partial x}(s^{(k)}) + \dfrac{\Delta t}{\varepsilon} \displaystyle\sum_{k=1}^{i} a_{i,k} h(s^{(k)}) \qquad i = 1, \ldots, \nu \\ s^{n+1} & = s^n - \Delta t \sum_{i=1}^{\nu} \tilde{b}_i \dfrac{\partial g}{\partial x}(s^{(i)}) + \dfrac{\Delta t}{\varepsilon} \displaystyle\sum_{i=1}^{\nu} b_i h(s^{(i)}) \end{cases}$$

Here $(\tilde{a}_{ik}, \tilde{b}_i)$ and (a_{ik}, b_i) are a pair of Butcher's tableaux of an explicit and a diagonally implicit RK. (For nonzero ε we need IMEX SSP)

Semidiscrete relaxed IMEX Runge-Kutta scheme

First step: $i = 1$

$$\begin{bmatrix} u^{(1)} \\ v^{(1)} \\ w^{(1)} \\ z^{(1)} \end{bmatrix} = \begin{bmatrix} u^{n} \\ v^{n} \\ w^{n} \\ z^{n} \end{bmatrix} + \frac{\Delta t}{\varepsilon} a_{1,1} g\left(\begin{bmatrix} u^{(1)} \\ v^{(1)} \\ w^{(1)} \\ z^{(1)} \end{bmatrix} \right) = \begin{bmatrix} u^{n} \\ v^{n} \\ w^{n} \\ z^{n} \end{bmatrix} + \frac{\Delta t}{\varepsilon} a_{1,1} \begin{bmatrix} 0 \\ -v^{(1)} + (\varepsilon\Phi^2 - 1) w_x^{(1)} \\ -w^{(1)} + p(u^{(1)}) \\ -z^{(1)} + v^{(1)} + f(u^{(1)}) \end{bmatrix}$$

we let $\varepsilon \to 0$ and therefore

$$u^{(1)} = u^n \qquad w^{(1)} = p(u^{(1)}) \qquad v^{(1)} = -w_x^{(1)} \qquad z^{(1)} = v^{(1)} + f(u^{(1)})$$

Second step: $i = 2$

$$s^{(2)} = s^n - \Delta t \tilde{a}_{2,1} g(s^{(1)})_x + \frac{\Delta t}{\varepsilon} a_{2,1} \underbrace{h(s^{(1)})}_{\equiv 0} + \frac{\Delta t}{\varepsilon} a_{2,2} h(s^{(2)})$$

$\varepsilon \to 0$ yields

$$\begin{cases} u^{(2)} = u^n - \Delta t \tilde{a}_{2,1} z_x^{(1)} \\ w^{(2)} = p(u^{(2)}) \\ v^{(2)} = -w_x^{(2)} \\ z^{(2)} = v^{(2)} + f(u^{(2)}) \end{cases}$$

Semidiscrete relaxed IMEX Runge-Kutta scheme

The semidiscrete relaxed scheme

The scheme reduces to an alternation of relaxation steps

$$h(s^{(i)}) = 0 \qquad \text{i.e.} \begin{cases} w^{(i)} = p(u^{(i)}) \\ v^{(i)} = -w_x^{(i)} \\ z^{(i)} = v^{(i)} + f(u^{(i)}) \end{cases}$$

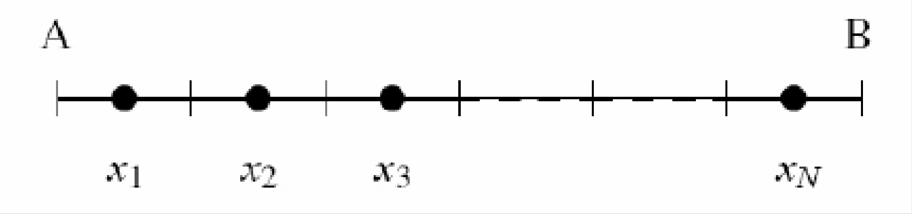
and transport steps where we advance for time $\tilde{a}_{i,k}\Delta t$

$$s_t + g(s)_x = 0$$

with initial data $s = s^{(i)}$, retain only the first component and assign it to $u^{(i+1)}$. Finally only the value of u^{n+1} is computed.

Fully discrete relaxed IMEX scheme: implicit part

Spatial discretization



- Introduce a (regular) grid with $x_j = a + h/2 + jh$ for $j = 1, \ldots, N$
- $h = (b-a)/N$
- $u_j^n = u(x_j, t^n)$, and denote $u^n = (u_j^n)_{j=1\ldots N}$, etc
- The implicit step can be treated using only function evaluations and matrix-vector multiplication

$$w^{(i)} = p(u^{(i)}) \qquad v^{(i)} = -\widehat{w_x^{(i)}} \qquad z^{(i)} = v^{(i)} + f(u^{(i)})$$

- Select a formula for the numerical gradient, to preserve stability and accuracy: Central finite differences formulas produce the most stable schemes.

Relaxed IMEX scheme: explicit part

Transport steps

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \\ w \\ z \end{pmatrix} + \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & \Phi^2 & 0 \\ 0 & 1 & 0 & 0 \\ A^2 & 0 & 0 & 0 \end{bmatrix} \frac{\partial}{\partial x}\begin{pmatrix} u \\ v \\ w \\ z \end{pmatrix} = 0$$

Diagonalization

Eigenvalues: $\pm\Phi, \pm A$
Characteristic variables :

$$U = \tfrac{1}{2}\left(Au + z\right),\ V = \tfrac{1}{2}\left(-Au + z\right),\ W = \tfrac{1}{2}\left(\tfrac{1}{\Phi}v + w\right),\ Z = \tfrac{1}{2}\left(-\tfrac{1}{\Phi}v + w\right),$$

$$\Longrightarrow \begin{array}{l} u_j^{(i)} = u_j^n - \Delta t \sum_{k=1}^{i-1} \tilde{a}_{i,k} A\left[\left(U_{j+1/2}^{(i)-} - U_{j-1/2}^{(i)-}\right) + \left(V_{j+1/2}^{(i)+} - V_{j-1/2}^{(i)+}\right)\right] \\ u_j^{n+1} = u_j^n - \lambda \sum_{i=1}^{\nu} \tilde{b}_i A\left[\left(U_{j+1/2}^{(i)-} - U_{j-1/2}^{(i)-}\right) + \left(V_{j+1/2}^{(i)+} - V_{j-1/2}^{(i)+}\right)\right] \end{array}$$

where $U_{j\pm1/2}^{(i)\pm}$ and $V_{j\pm1/2}^{(i)\pm}$ are suitable non-oscillatory reconstructions.

Von Neumann stability analysis

Linear stability

On higher order schemes, we studied stability linearizing both the equation and the scheme and computing the amplification factors of each Fourier mode in a VonNeumann analysis. We obtain a timestep restriction like

$$\Delta \mathrm{t} \leq \frac{C_1}{D}(1-\alpha h \Phi)h^2 + \frac{C_2}{\mu}h$$

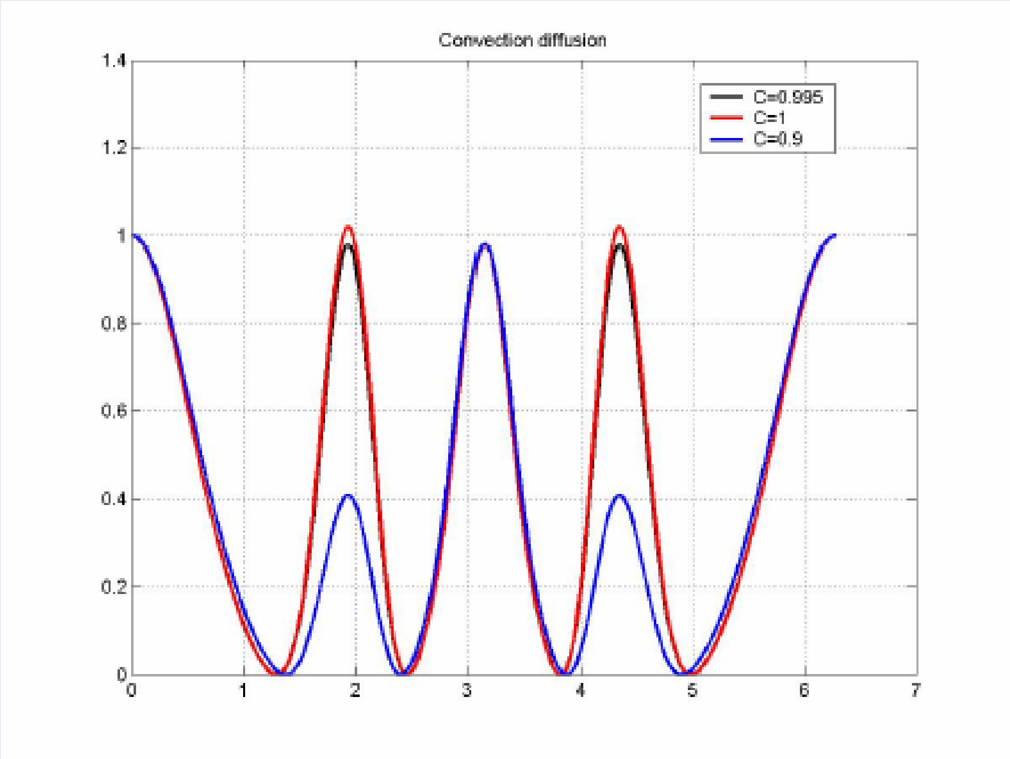
Diffusive regime $D > \mu h$

The parabolic CFL is dominant and we have C_1 as in the following table:

	RK1	RK2	RK3
P-wise constant	2	2	2.51
P-wise linear	0.94	0.94	1.18
linearized WENO5	0.79	0.79	1

Von Neumann stability analysis

Amplification factor, WENO5 RK3 $D = 1$ $\mu = 1$ $h = 0.01$



Hyperbolic regime $D = 0$

The subcharacteristic condition $A \geq |f'(u)|$ holds

Conclusions

$$-\epsilon u'' + u' = 1$$
$$u(0) = u(1) = 0$$

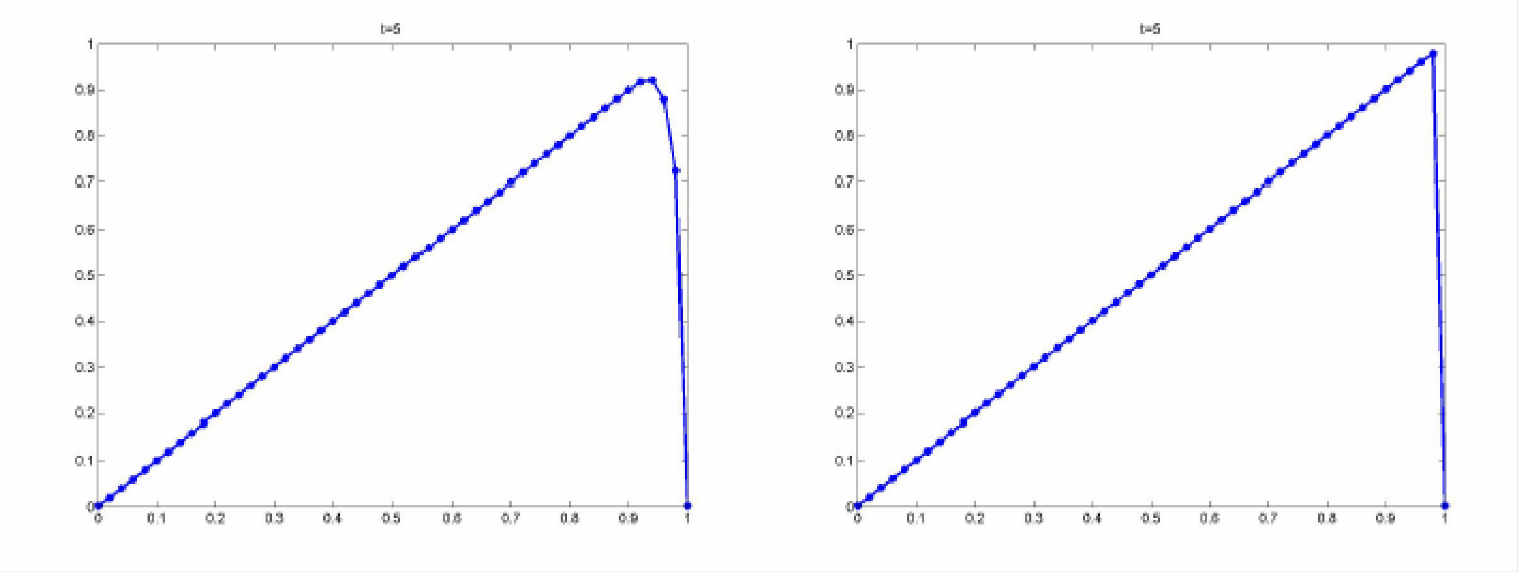


Figura: Solution obtained as steady state with ENO reconstructions of order 2, $N = 50$ coupled with second order Dirichlet boundary conditions: left $\epsilon = 10^{-2}$, right $\epsilon = 10^{-4}$.

F. Cavalli, PhD Thesis, to appear, 2006