Mixed Finite Element Methods for Non-Linear Fokker-Planck Equations

Martin Burger[1] Jose Carrillo[2] Marie-Therese Wolfram[3]

[1]Westfälische Wilhelms-Universität Münster

[2]Universitat Autonoma de Barcelona

[3]RICAM, Austrian Academy of Sciences

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Outline

Non-Linear Fokker-Planck Equations I

Consider the following minimization problem:

Given a density ρ_{n-1}, find ρ_n such that

$$\inf_{\rho,\rho_n,u}\left(E(\rho_n)+\int_{t_{n-1}}^{t_n}\int_{\mathbb{R}^d} c\left(u\left(x,t\right)\right)\rho\left(x,t\right)dxdt\right)$$

under the constraint that

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho u)=0$$

$$\rho(\cdot,t_{n-1})=\rho_{n-1},\quad \rho(\cdot,t_n)=\rho_n.$$

Non-Linear Fokker-Planck Equations II

The optimality condition for the minimization problem is given by

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left[\rho \left(\nabla c^*\right) \left(\nabla \frac{\delta E}{\delta \rho}\right)\right]$$
$$\rho(x,0) = \rho_0(x).$$

with no-flux boundary conditions. The energy E is given by

$$E = \underbrace{\mathcal{U}}_{\text{internal energy}} + \underbrace{\mathcal{V}}_{\text{potential energy}} + \underbrace{\mathcal{W}}_{\text{interaction energy}}$$

$$\mathcal{U}(\rho) = \int_{\mathbb{R}^n} U\left(\rho\left(x\right)\right) dx$$
$$\mathcal{V}(\rho) = \int_{\mathbb{R}^n} \rho(x)V(x)dx$$
$$\mathcal{W}(\rho) = \frac{1}{2}\int_{\mathbb{R}^n \times \mathbb{R}^n} W(x-y)\rho(x)\rho(y)dxdy$$

Quadratic Cost

Classical examples with cost functional $c(x) = \frac{|x|^2}{2}$

$U(s) = s \log s, \ V = 0, \ W = 0$	heat equation
$U(s) = \frac{s^m}{m-1}, \ V = 0, \ W = 0$	porous-medium type equation
$U(s) = s \log s$, V given potential	linear Fokker-Planck equation
$U = 0, \ V = 0, \ W(z) = \frac{\lvert z\rvert}{3}$	model for granular flow
$W(z)$ non-local kernel	continuous swarming models

The relativistic cost is given by

$$c(x) = \begin{cases} 1 - \sqrt{1 - \frac{1}{c^2}|x|^2} & |x| < c \\ \infty & |x| \geq c \end{cases}$$

where $c > 0$ can be interpreted as a maximal speed.
The corresponding optimality condition with $U(s) = s\log(s) - s$ is the so-called relativistic heat equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\frac{\rho \nabla \rho}{\sqrt{\rho^2 + \frac{1}{c^2}|\nabla \rho|}} \right)$$

The cost functional $c(x) = \frac{|x|^p}{p}$ gives the well-known p-Laplace equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(|\nabla \rho|^{p-2} \nabla \rho \right).$$

Linearization I

Consider the linearized minimization problem

Given a density ρ_{n-1}, find ρ_n such that

$$\inf_{\rho,\rho_n,u}\left(E(\rho_n)+\int_{t_{n-1}}^{t_n}\int_{\mathbb{R}^d}c\left(u\left(x,t\right)\right)\rho_{n-1}\left(x,t\right)dxdt\right)$$

under the constraint that

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho_{n-1}u)=0$$

$$\rho(\cdot,t_{n-1})=\rho_{n-1},\quad \rho(\cdot,t_n)=\rho_n.$$

The optimality condition is given by

$$\frac{\partial\rho}{\partial t}=\mathrm{div}\left(\rho_{n-1}\nabla\left(\frac{\partial E}{\partial\rho}\right)\right)$$

$$\rho(x,0)=\rho_0(x)$$

and no flux boundary conditions.

We introduce the new variables

$$\mu = \frac{\delta E}{\delta \rho} \qquad \text{and} \qquad \mathbf{j} = \rho_{n-1} \nabla \mu$$

We replace the time derivative by a finite difference quotient and obtain:

$$\mu_n = \frac{\delta E}{\delta \rho_n}(\rho_n)$$
$$\rho_n - \sqrt{\tau}\,\mathrm{div}\,\mathbf{j}_n = \rho_{n-1}$$
$$\sqrt{\tau}\nabla \mu_n - \frac{1}{\rho_{n-1}}\mathbf{j}_n = 0$$

Problem is still non-linear, therefore we linearize E, for example

$$E(\rho_n) = \rho_n \log \rho_n \qquad \tilde{E}(\rho_n) = \rho_n \left(\log \rho_{n-1} + \frac{\rho_n - \rho_{n-1}}{\rho_{n-1}} \right)$$

Proposition

Let $0 < c_1 \leq \rho_{n-1}(x) \leq c_2$ *for all* $x \in \Omega$. *Then the solution* ρ_n *of*

$$\rho_n - \sqrt{\tau}\,\text{div}\,\mathbf{j}_n = \rho_{n-1}$$
$$\sqrt{\tau}\nabla\mu_n - \frac{1}{\rho_{n-1}}\mathbf{j}_n = 0.$$

with $\mu_n = \frac{\delta E}{\delta \rho_n}(\rho_n)$ *satisfies*

$$c_1 \leq \rho_n(x) \leq c_2 \quad \forall x \in \Omega.$$

Long time behavior of the Fokker-Planck Equation: Linearization with $\mu = \frac{\delta E}{\delta \rho_n}$ guarantees decay of the numerical entropy, using a similar argument as in

- A. Arnold, A. Unterreiter, *Entropy Decay of Discretized Fokker-Planck Equations I - Temporal Semi-Discretization*, Comp. Math. Appl. 46, No. 10-11, 2003

Then the weak formulation is given by

Find $\rho_n, \mu_n \in L^2(\Omega)$ and $\mathbf{j}_n \in H(\mathrm{div}, \Omega)$ such that:

$$\int_\Omega a(\rho_{n-1})\rho v dx + \int_\Omega \mu_n v dx = \int_\Omega f(\rho_{n-1}) v dx \qquad \forall v \in L^2(\Omega)$$

$$\int_\Omega \rho_n w dx - \int_\Omega \sqrt{\tau}\, \mathrm{div}\, \mathbf{j}_n w \; dx = \int_\Omega \rho_{n-1} w dx \qquad \forall w \in L^2(\Omega)$$

$$-\int_\Omega \sqrt{\tau}\mu_n \,\mathrm{div}\, \mathbf{q} dx - \int_\Omega \frac{1}{\rho_{n-1}} \mathbf{j}_n \mathbf{q} dx = 0 \qquad \forall \mathbf{q} \in H(\mathrm{div}, \Omega)$$

Abstract formulation: Find $u \in V$ and $p \in Q$ solutions of

$$a(u, v) + b(v, p) = \langle f, v \rangle \quad \forall\, v \in V$$
$$b(u, q) - c(p, q) = \langle g, q \rangle \quad \forall\, q \in Q.$$

where a, b, c are continuous bilinear forms.

Existence and Uniqueness

If the following conditions hold:

- a is a bounded and coercive, i.e.

$$
\begin{aligned}
& & |a(u,v)| \le \|a\|\|u\|_V\|v\|_V & \qquad \forall\ u,v \in V \\
\exists\ \alpha > 0 & & a(v,v) \ge \alpha\|v\|_V^2 & \qquad \forall\ v \in V_0
\end{aligned}
$$

  with $V_0 = \{v \in V|\ b(v,p) = 0\ \forall p \in Q\}$,

- b is bounded and satisfies the inf-sup-condition, i.e.

$$
\begin{aligned}
& & |b(v,q)| \le \|b\|\|v\|_V\|q\|_Q & \qquad \forall v \in V,\ q \in Q \\
\exists\ \beta > 0 & & \sup_{v\in V} \frac{b(v,q)}{\|v\|_V} \ge \beta\|q\|_Q & \qquad \forall p \in Q
\end{aligned}
$$

- c is bounded and coercive, i.e.

$$
\begin{aligned}
& & |c(p,q)| \le \|c\|\|\,\|_Q\|q\|_Q & \qquad \forall p,q \in Q \\
\exists\ \gamma > 0 & & c(q,q) \ge \gamma\|q\|_Q^2 & \qquad \forall q \in Q
\end{aligned}
$$

Then the system has a unique solution.

Properties of $H(\mathrm{div}, \Omega)$ and $L^2(\Omega)$:

- $\sigma \in H(\mathrm{div}, \Omega) \Rightarrow \sigma \cdot n$ has to be continuous
- $v \in L^2(\Omega) \Rightarrow$ no continuity requirements

The cheapest $H(\mathrm{div}, \Omega)$ conforming finite element is the Raviart Thomas element defined by

$$V_h = \left\{ \begin{pmatrix} a \\ b \end{pmatrix} + c \begin{pmatrix} x \\ y \end{pmatrix} : a, b, c \in \mathbb{R} \right\}$$

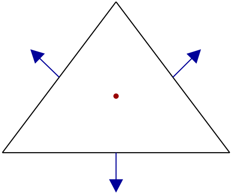
Degrees of freedom are associated to the edges e_i of the triangle:

$$\int_{e_i} \phi_j \cdot \mathbf{n}_{e_i} ds = \delta_{i,j} \quad i = 1, 2, 3$$

The lowest order $L^2(\Omega)$ conforming finite element space Q_h contains the element-wise constant functions.

Low Order Raviart-Thomas Elements

Degrees of freedom:



- ρ, μ
- $\mathbf{j}$

The De-Rham sequence:

$$\begin{array}{ccc} H(\mathrm{div}, \Omega) & \xrightarrow[\mathrm{div}]{} & L^2(\Omega) \\ \downarrow I_h & & \downarrow P_h \\ V_h & \xrightarrow[\mathrm{div}]{} & Q_h \end{array}$$

Patlak-Keller-Segel Model I

PKS Model is used for describing the motion of cells attracted by a self-emitted chemical substrate.

$$
\begin{aligned}
& -\Delta c - \rho = -\langle \rho \rangle \\
& \rho_t = \operatorname{div}\left(\rho \nabla \left(\log \rho - \chi c\right)\right) \\
& \rho(x, 0) = \rho_0(x) \geq 0
\end{aligned}
$$

with no-flux boundary conditions. Here

- c denotes the concentration of the chemo-attractant
- ρ represents the cell density and
- χ is the sensitivity of the bacteria to the chemo-attractant.

Patlak-Keller-Segel Model II

Total mass of system:

$$M := \int_{\mathbb{R}^2} \rho_0 dx = \int_{\mathbb{R}^2} \rho(x,t) dx.$$

Blow up behavior for $\chi M > M_C$,

$$M_c = \begin{cases} 8\pi & \text{for unbounded domains } \Omega \subset \mathbb{R}^2 \\ 4\pi & \text{for bounded, connected domains } \Omega \subset \mathbb{R}^2 \end{cases}$$

- A. Blanchet, J. A. Carrillo and N. Masmoudi, *Infinite Time Aggregation For The Critical Patlak-Keller-Segel Model in* $\mathbb{R}^2$, Preprint UAB
- V. Calvez and J. A. Carrillo, *Volume effects in the Keller-Segel model: energy estimates preventing blow up*, Journal Mathématiques Pures et Appliquées 86, 155-175, 2006

Mixed Finite Element Method I

We introduce new variables

- Concentration gradient: $\mathbf{e} = \nabla c$
- Flux: $\mathbf{j} = \rho \nabla \mu$ with $\mu = \frac{\delta E}{\delta \rho} = \log \rho - \chi c$

and the following linearization $\mu \approx \log \rho_{n-1} + \frac{\rho_n - \rho_{n-1}}{\rho_{n-1}} - \chi c$.

Find $c, \rho_n, \mu_n \in L^2(\Omega)$ and $\mathbf{e}, \mathbf{j}_n \in H(\mathrm{div}, \Omega)$ such that

$$-\int_\Omega \mathbf{e} \cdot \mathbf{p} dx + \int_\Omega c \,\mathrm{div}\, \mathbf{p} dx = 0 \qquad \forall \mathbf{e} \in H(\mathrm{div}, \Omega)$$

$$\int_\Omega \mathrm{div}\, \mathbf{e} r dx - \int_\Omega \rho_n r dx = -\int_\Omega \langle \rho_0 \rangle r dx \qquad \forall r \in L^2(\Omega)$$

$$-\int_\Omega \chi c u dx + \int_\Omega \frac{\rho_n}{\rho_{n-1}} u dx - \int_\Omega \mu_n u dx = -\int_\Omega \left(\log \rho_{n-1} + 1\right) u dx \qquad \forall u \in L^2(\Omega)$$

$$-\int_\Omega \rho_n v dx + \int_\Omega \sqrt{\tau}\, \mathrm{div}\, \mathbf{j}_n v dx = -\int_\Omega \rho_{n-1} v dx \qquad \forall v \in L^2(\Omega)$$

$$\int_\Omega \sqrt{\tau} \mu_n \,\mathrm{div}\, \mathbf{q} dx + \int_\Omega \frac{1}{\rho_{n-1}} \mathbf{j}_n \cdot \mathbf{q} dx = 0 \qquad \forall \mathbf{q} \in H(\mathrm{div}, \Omega).$$

- Initial density:

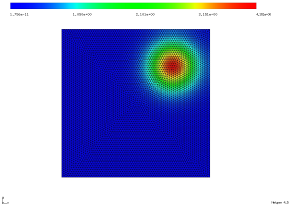
$$\rho_0(x, y) = \frac{c}{2\pi} e^{-\frac{(x-x_0)^2+(y-y_0)^2}{2}}$$

- Domain: Square of size $[-5, 5] \times [-5, 5]$ with discretization of 10348 triangles
- Hp-mesh refinement in corner of expected blow up
- replace

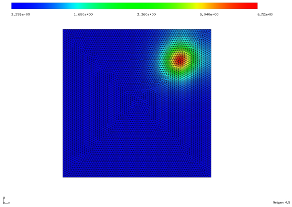
$$\frac{1}{\rho_{n-1}} \approx \frac{1}{\max(\rho_{n-1}, h)}$$

where h is the mesh size

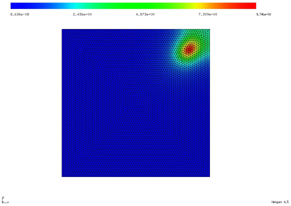
Evolution of ρ with mass $M = 10\pi$



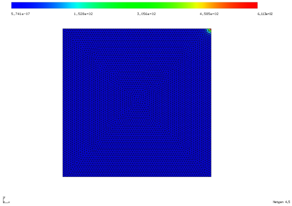
(a) $t = 0$



(b) $t = 0.4$

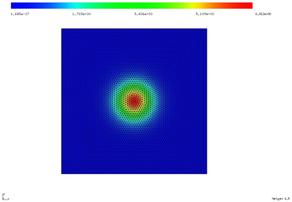


(c) $t = 0.8$

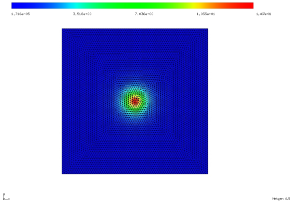


(d) $t = 1.4$

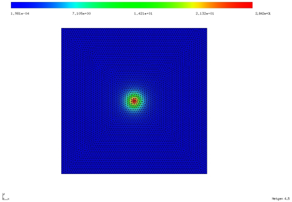
Evolution of ρ with mass $M = 10\pi$



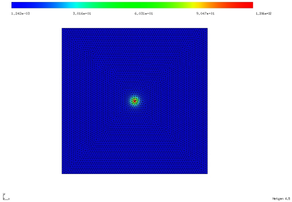
(e) $t = 0$



(f) $t = 0.4$

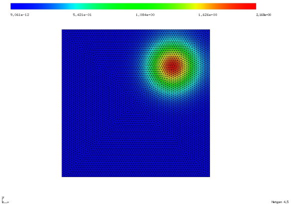


(g) $t = 0.8$

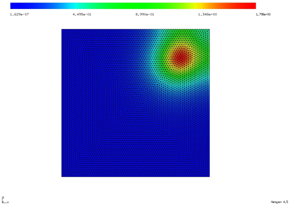


(h) $t = 1.4$

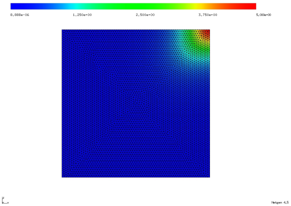
Evolution of ρ with mass $M = 6\pi$



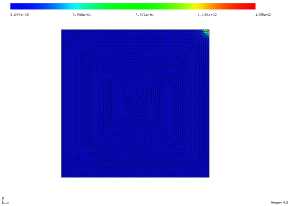
(i) $t = 0$



(j) $t = 0.4$

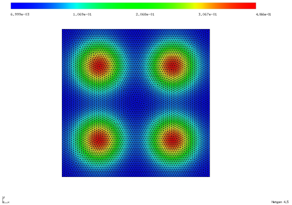


(k) $t = 0.8$

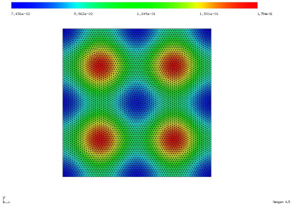


(l) $t = 1.4$

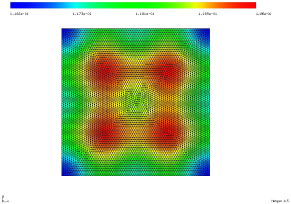
Evolution of 4 densities ρ_i with masses $m_i = 0.9\pi$



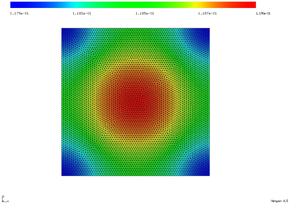
(m) $t = 0$



(n) $t = 1$



(o) $t = 4$



(p) $t = 6$

Figure: Evolution of four densities ρ with four masses $m_i = 0.9\pi$

We consider the porous medium type equations

$$\rho_t = \mathrm{div}\,(\nabla \rho^m) = \mathrm{div}\left(\frac{m}{m-1}\rho\nabla\rho^{m-1}\right)$$
$$\rho(x,0) = \rho_0(x)$$

for $m \geq 2$ with homogenous Neumann boundary conditions. For $m < 1$ this equation is known as the Fast Diffusion Equation (FDE).

Applications:

- Flow of a gas through a porous medium for $m > 2$,
- thin films with no surface tension for $m = 4$,
- and many other applications in physics ...

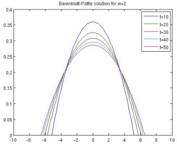
J. L. Vazquez, *The Porous Medium Equation*, Oxford University Press

Barenblatt-Pattle Solutions

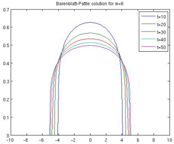
Solution of the porous medium equation is given by the Barenblatt-Pattle profile

$$V(|x|,t) = t^{-kN}\left(C_1 - \frac{k\,(m-1)}{2m}|x|^2 t^{-2k}\right)_+^{\frac{1}{m-1}}$$

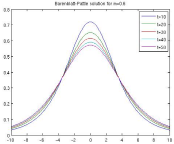
where $k = (N(m-1)+2)^{-1}$.



(a) $m = 2$



(b) $m = 6$



(c) $m = 0.6$

Linearization of Porous Medium Equations

Introduce a new variable

$$\mu = \frac{m}{m-1}\rho^{m-1}$$
$$\approx \frac{m}{m-1}\left(\rho_{n-1}^{m-1} + (m-1)\,\tilde{\rho}^{m-2}\,(\rho - \rho_{n-1})\right)$$

The flux is given by

$$\mathbf{j} = \rho\nabla\mu \approx \rho_{n-1}\nabla\mu.$$

The linearized system then reads as

$$m\rho_{n-1}^{m-2}\rho_n - \mu_n = -\frac{m(m-2)}{m-1}\rho_{n-1}^{m-1}$$
$$-\rho_n + \sqrt{\tau}\,\mathrm{div}\,\mathbf{j}_n = -\rho_{n-1}$$
$$-\sqrt{\tau}\nabla\mu_n + \frac{1}{\rho_{n-1}}\mathbf{j}_n = 0.$$

The variational formulation is given by:

Find $\rho_n, \mu_n \in L^2(\Omega)$ and $\mathbf{j}_n \in H(\text{div}, \Omega)$ such that

$$\int_\Omega m\rho_{n-1}^{m-2}\rho_n\omega dx - \int \mu_n\omega dx = -\int \frac{m(m-2)}{m-1}\rho_{n-1}^{m-1}\omega dx \qquad \text{for all } \omega \in L^2(\Omega)$$

$$-\int_\Omega \rho_n\xi dx + \int \sqrt{\tau}\,\text{div}\,\mathbf{j}_n\xi dx = -\int \rho_{n-1}\xi dx \qquad \text{for all } \xi \in L^2(\Omega)$$

$$\int_\Omega \sqrt{\tau}\mu_n\,\text{div}\,\theta + \int \frac{1}{\tilde{\rho}}\mathbf{j}\theta dx = 0 \qquad \text{for all } \theta \in H(\text{div}, \Omega)$$

For the numerical computations we

- replace

$$\frac{1}{\rho_{n-1}^{2-m}} \approx \frac{1}{\max(\rho_{n-1}, h)^{2-m}}$$

  where h is the mesh size

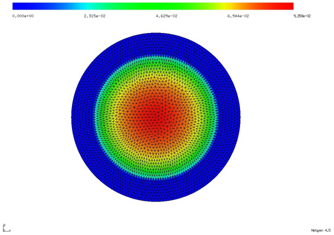
- and do a back-projection after each time step

$$\rho = max(\rho, 0).$$

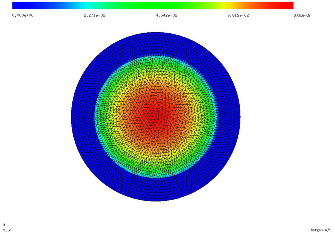
Problem Setup:

- Circle of radius $r = 2$
- Time steps: $\tau = 10^{-1}$ for PME, $\tau = 10^{-3}$ for FDE
- Initial Guess: Barenblatt Profile at $t = 0.1$

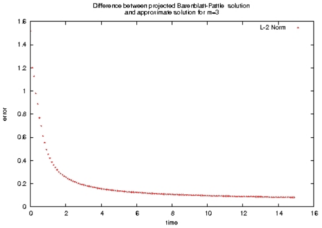
Numerical Simulation for $m = 3$



(d) $t = 15$

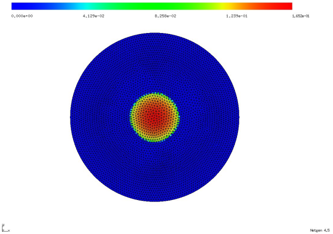


(e) $t = 15$

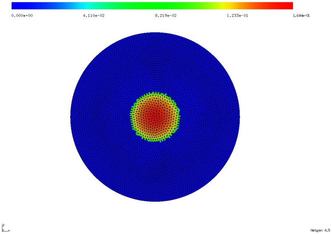


(f) Difference of the approximated solution to the BP solution in L^2 norm

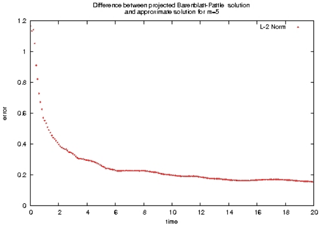
Numerical Simulation for $m = 5$



(g) $t = 20$

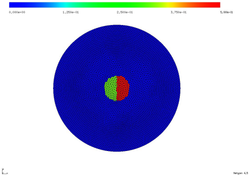


(h) $t = 20$

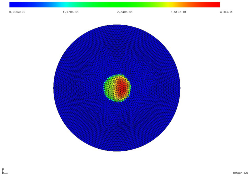


(i) Difference of the approximated solution to the BP solution in L^2 norm

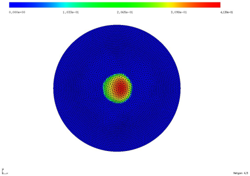
Numerical Simulation for $m = 3$



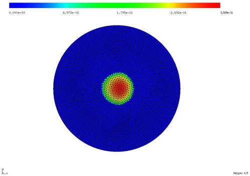
(j) $t = 0$



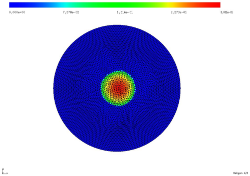
(k) $t = 0.1$



(l) $t = 0.25$

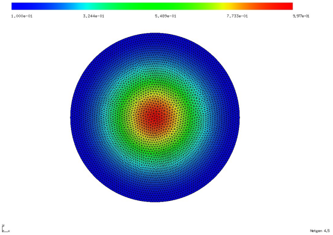


(m) $t = 0.5$

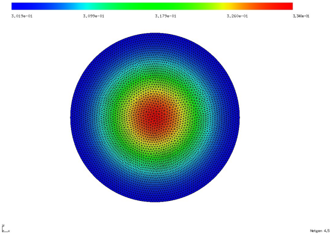


(n) $t = 1$

Numerical Simulation for $m = 0.8$



(o) $t = 1$



(p) $t = 2$

Relativistic Heat Equation I

Relativistic heat equation (RHE) is given by

$$\frac{\partial \rho}{\partial t} = \nu \,\mathrm{div}\left(\frac{\rho \nabla \rho}{\sqrt{\rho^2 + \frac{\nu^2}{c^2} |\nabla \rho|^2}} \right)$$
$$\rho(x, 0) = \rho_0(x)$$

where $\nu > 0$ is a constant representing a kinematic viscosity and c is the speed of light.
Asymptotic behavior :

- For $c \to \infty$ the solutions of the RHE converge to the solution of the heat equation $\rho_t = \nu \Delta \rho$.
- For $\nu \to \infty$ the solutions of the RHE converge to the solution of

$$\frac{\partial \rho}{\partial t} = c \,\mathrm{div}\left(\rho \frac{\nabla \rho}{|\nabla \rho|} \right).$$

Relativistic Heat Equation II

The solution of the limiting equation with initial data $\rho_0(x) = \alpha\chi_C(x),\ \alpha > 0$ is given by

$$\rho(x,t) = \alpha \frac{|C|}{|C(t)|}\chi_{C(t)}(x)$$

where

$$C(t) := \{x \in \mathbb{R}^N : d(x,C) \le t\}.$$

For further information

- F. Andreu, V. Caselles, J.M. Manzon and S. Moll, *On The Relativistic Heat Equations And An Asymptotic Regime Of It*, Preprint
- V. Caselles, *Convergence Of The Relativistic Heat Equations To The Heat Equations As* $c \to \infty$, Publ. Mat. 51 (2007), 121-142
- R. J. McCann, M. Puel, *Constructing A Relativistic Heat Flow By Transport Time Steps*

Relativistic Heat Equation III

Consider

$$\frac{\partial \rho}{\partial t} = \nu \operatorname{div} \left(\frac{\nabla \rho}{\sqrt{1 + \frac{\nu^2}{c^2} \frac{|\nabla \rho|^2}{\rho^2}}} \right)$$

and introduce new variables $\mu = \log \rho$ and the flux $\mathbf{j} = \rho \nabla \mu$. Using the same linearization as for the Keller-Segel model we obtain

$$\begin{aligned} \frac{1}{\rho_{n-1}} \rho_n - \mu_n &= 1 - \log \rho_{n-1} \\ -\rho_n + \sqrt{\tau} \operatorname{div} \mathbf{j}_n &= -\rho_{n-1} \\ \frac{\sqrt{\tau}}{\sqrt{1 + |\nabla \mu_{n-1}|^2}} \nabla \mu_n + \frac{\mathbf{j}_n}{\rho_{n-1}} &= 0 \end{aligned}$$

Problem: Higher order basis functions for μ

Introduce a new variable $\sigma = \rho_x$ - then the linearized system is given by

$$\sigma - \rho_x = 0$$

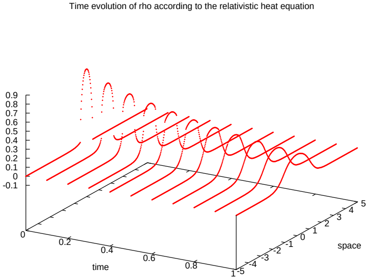
$$-\frac{\partial \rho}{\partial t} + \partial_x \left(\frac{\sigma}{\sqrt{1 + \frac{\nu^2}{c^2} \frac{|\tilde{\sigma}|^2}{\tilde{\rho}^2}}} \right) = 0.$$

Find $\sigma \in L^2(\Omega)$ and $\rho \in H^1(\Omega)$ such that

$$\int \sigma \omega dx - \int \rho_x \omega dx = 0 \qquad \text{for all } \omega \in L^2(\Omega)$$

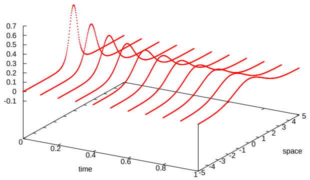
$$-\int \frac{1}{\sqrt{1 + \frac{\nu^2}{c^2} \frac{|\tilde{\sigma}|^2}{\tilde{\rho}^2}}} \sigma \xi_x dx - \int \frac{1}{\tau} \rho \xi dx = -\int \frac{1}{\tau} \tilde{\rho} \xi dx \qquad \text{for all } \xi \in H^1(\Omega).$$

Relativistic Heat Equation
$c = 1.0$ and $\nu = 1.0$

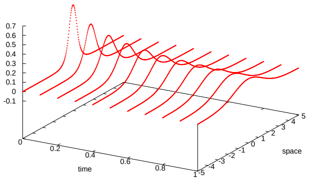


Relativistic Heat Equation
$c = 1e10$ and $\nu = 1.0$

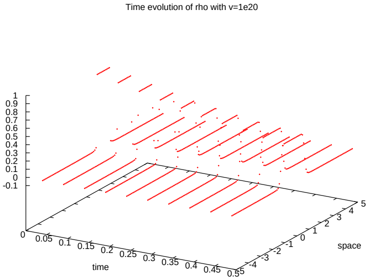
Time evolution of rho according to the relativistic heat equation



Time evolution of rho according to the heat equation



Relativistic Heat Equation
$c = 1.0$ and $\nu = 1e20$



Exact Solution: $\rho(x, 0.5) = \frac{1}{2}\chi_{[-1,1]}$

- Extension of the numerical scheme to use higher order basis functions
- Long-time behavior of numerical scheme
- Newton method after linearization of Wasserstein distance

Software: NETGEN/NGSolve developed by Joachim Schöberl, RWTH Aachen

Thank you very much for your attention !

What's still left to do

- Extension of the numerical scheme to use higher order basis functions
- Long-time behavior of numerical scheme
- Newton method after linearization of Wasserstein distance

Software: NETGEN/NGSolve developed by Joachim Schöberl, RWTH Aachen

Thank you very much for your attention !