Numerical schemes for kinetic equations with anomalous diffusion scaling:
Heavy tail equilibria and degenerate collision frequencies

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Outline

Main motivations of multi-scale numerical schemes

Concerned problems

- $\mathcal{P}^\varepsilon$ is a stiff problem having an asymptotic $\mathcal{P}^0$ when $\varepsilon \to 0$. Solving it directly would require the adaptation of the numerical parameters $h = O(\varepsilon^\alpha)$. Impossible in practice for small ε.
- ε may depend on space (or on time). Decomposition domain methods face the delicate problem of handling the interfaces.

Desired properties

- Uniform accuracy with respect to ε, without increasing computational cost

$$\sup_{\varepsilon \in [0,1]} \|f_h^\varepsilon - f^\varepsilon\| \leq Ch^m.$$

  m is the order in time of the numerical method.
- Weaker property, Asymptotic preserving property:
  - For fixed $\varepsilon > 0$, $\|f_h^\varepsilon - f^\varepsilon\| \to 0$ when $h \to 0$.
  - For fixed h, $f_h^\varepsilon \to f_h^0$ when $\varepsilon \to 0$, with $\|f_h^0 - f^0\| \to 0$ when $h \to 0$.
- Reduce the numerical cost when $\varepsilon \to 0$.

Why uniformly accurate AP schemes may be needed

- A usual argument (see Golse-Jin-Levermore) says that Unif. convergence when $\varepsilon \to 0 \Longrightarrow$ Unif. convergence of when $\Delta t \to 0$. For most of the AP schemes, the uniform (in ε) numerical order is *smaller* than the pointwise (fixed ε) numerical order.
- This is due to a possible slow convergence in ε to the asymptotic model:
  - Continuous level:
  $$\|f^\varepsilon - f^0\| \simeq \varepsilon^\gamma \quad \text{with small } \gamma.$$
  This is the case for anomalous diffusion asymptotics.
  - Discrete level:
  $$\sup_{h\in[0,1]} \|f_h^\varepsilon - f_h^0\| \simeq \varepsilon^\delta \quad \text{with } \delta \leq \gamma.$$
- The consistency error of a (non UA) has the generic form
$$\|f_h^\varepsilon - f^\varepsilon\| \simeq \frac{h^m}{\varepsilon^q}.$$
- The resulting error is at least
$$\|f_h^\varepsilon - f^\varepsilon\| \simeq \min\left(\frac{h^m}{\varepsilon^q} + h^m, \varepsilon^\delta\right) = h^{\frac{\delta}{\delta+q}\cdot m}.$$

Diffusion scaling

Diffusion description occurs when the particles interact (collisions for instance with some media) with a small mean free path.

$$\partial_t f + \frac{1}{\varepsilon} v \cdot \nabla_x f = \frac{1}{\varepsilon^2} Lf.$$

- L is a linear collision operator with a one dimensional kernel

$$\mathrm{Ker}L = \mathrm{Span}\{M(v)\}, \quad \langle M \rangle = 1, \quad \langle vM \rangle = 0, \quad \langle v \otimes vM \rangle < \infty.$$

- the simplest example:

$$Lf(v) = \rho(t,x)M(v) - f, \qquad \rho(t,x) = \int_{\mathbb{R}^d} f(t,x,v)dv.$$

$$M(v) = \frac{1}{(2\pi)^{d/2}} \exp(-|v|^2/2).$$

Diffusion limit

If $\varepsilon \to 0$, then $f^\varepsilon \to \rho M$ with

$$\partial_t \rho = \nabla_x \cdot (D \nabla_x \rho) \,, \qquad D = \langle v \otimes L^{-1}(vM) \rangle .$$

with suitable space boundary conditions. See: Degond-Goudon-Poupaud (2000).

Asymptotic Preserving (AP) numerical schemes:

Well developed now in collisional kinetic theory, plasmas physics, radiative transfer:
Gabetta-Pareschi-Toscani 97, Klar 99, Jin-Pareschi-Toscani 00, Pareschi-Russo 00', Crispel-Degond-Vignal 07, Carillo-Goudon-Lafitte, L-Mieussens 08, Filbet-Jin 10, Dimarco-Pareschi 11, Degond-Lozinski-Narski-Negulescu 12, L-Crouseilles 12,L-Méhats 12, Buet-Després-Franck 12 ...

Anomalous diffusion scaling - heavy tail equilibrium

- The diffusion scaling does not capture a non trivial macroscopic dynamics when the equilibrium $M(v)$ has a heavy tail:

$$M(v) = \frac{m}{1+|v|^\beta}, \quad v \in \mathbb{R}^d, \quad , d < \beta < d+2.$$

Astrophysical plasmas, granular and porous media, Levy process (random walk with heavy-tail distribution) and fractional Brownian motion, economy and social sciences (Pareto distributions), ...

- Reason:

$$\langle M \rangle = 1, \quad \langle vM \rangle = 0, \quad \langle v \otimes vM \rangle = \infty.$$

- The suitable scaling is

$$\partial_t f + \varepsilon^{1-\alpha} v \cdot \nabla_x f = \varepsilon^{-\alpha} Lf, \qquad \alpha = \beta - d \in (0,2).$$

The asymptotics $\varepsilon \to 0$ is called: the anomalous diffusion limit.

Anomalous diffusion scaling - Singular collision frequency

- Anomalous diffusion may also happen when the collision frequency $\nu(v)$ degenerates at $v = 0$:

$$Lf(v) = \nu(v)\left(\rho_f M(v) - f\right), \qquad \rho_f = \frac{\langle \nu(v) f(v) \rangle}{\langle \nu(v) M(v) \rangle}$$

where M is taken constant near $v = 0$ and

$$\langle \frac{v \otimes v}{\nu(v)} M(v) \rangle = \infty.$$

The effect of small velocities.

- Example:

$$\nu(v) = \nu_0 |v|^{d+2+\beta}, \text{ near } v = 0, \ \beta > 0.$$

- The suitable scaling is

$$\partial_t f + \varepsilon^{1-\alpha} v \cdot \nabla_x f = \varepsilon^{-\alpha} Lf, \qquad \alpha = \frac{2d+2+\beta}{d+1+\beta} \in (1,2)$$

Anomalous diffusion: some references

- Kleiber and Cost: Statistical size distributions in economic and actuarial sciences (2003).
- Mathematics literature: Bensoussan-Lions-Papanicolaou (1979), Phd of De Moor (Rennes, limites diffusives des équations cinétiques stochastiques) Mellet (2009), Mellet-Mischler-Mouhot (2011), Ben Abdallah-Mellet-Puel (2011,2012)

A unified framework

$$\langle \frac{v \otimes v}{\nu(v)} M(v) \rangle = \infty,$$

either because of large velocities (heavy-tail equilibrium) or because of small velocities (singular frequency).

Using space Fourier variable

$$\partial_t \widehat{f} + \varepsilon^{1-\alpha} ik \cdot v \widehat{f} = \varepsilon^{-\alpha} \nu (\widehat{\rho} M - \widehat{f}).$$

$$\widehat{f} = \frac{\nu M}{\nu + i\varepsilon k \cdot v} \widehat{\rho} - \varepsilon^{\alpha} \frac{\partial_t \widehat{f}}{\nu + i\varepsilon k \cdot v}$$

$$\partial_t \widehat{\rho} + \varepsilon^{1-\alpha} \left\langle \frac{ik \cdot v \, \nu M}{\nu + i\varepsilon k \cdot v} \right\rangle \widehat{\rho} = O(\varepsilon^{\gamma})$$

One has to compute

$$D(k) = \lim_{\varepsilon \to 0} \varepsilon^{1-\alpha} \left\langle \frac{ik \cdot v \, \nu M}{\nu + i\varepsilon k \cdot v} \right\rangle = \lim_{\varepsilon \to 0} \varepsilon^{2-\alpha} \left\langle \frac{(k \cdot v)^2 \, \nu M}{\nu^2 + (\varepsilon k \cdot v)^2} \right\rangle$$

- Normal diffusion: $\alpha = 2$, $C = \langle v \otimes vM/\nu \rangle < +\infty$.

$$D(k) = C|k|^2.$$

- Anomalous diffusion: $\langle v \otimes vM/\nu \rangle = +\infty$.

Large velocities effect

- Heavy-tail equilibrium, large velocities effect: $\nu \equiv 1$ and M is a Maxwellain. Change of variables: $w = \varepsilon|k|v$

$$D(k) = C_{d,\alpha}|k|^{\alpha}, \qquad C_{d,\alpha} = \left\langle \frac{m(u\cdot w)^2}{(1+(u\cdot w)^2)|w|^{\beta}} \right\rangle, \qquad u \in \mathbb{S}^{d-1}.$$

- Degenrate collision frequency, small velocities effect: $M = M_0$ and $\nu(v) = \nu_0|v|^{d+2+\beta}$. Change of variable: $w = \frac{\varepsilon|k|v}{\nu(v)}$.

$$D(k) = C_{d,\alpha}|k|^{\alpha}, \qquad C_{d,\alpha} = \frac{M_0\nu_0^{1-\alpha}}{d+1+\beta}\left\langle \frac{1}{|w|^{d+\alpha}} \frac{(w\cdot u)^2}{1+(w\cdot u)^2} \right\rangle$$

- In the original (non Fourier) variables, it is a non local operator

$$D = C_{d,\alpha}(-\Delta)^{\alpha/2}.$$

$$(-\Delta)^{\alpha/2}\rho(x) = PV\int_{\mathbb{R}^d} \frac{\rho(x+y)-\rho(y)}{|y|^{\alpha+d}}dy.$$

If ρ is smooth then

$$(-\Delta)^{\alpha/2}\rho(x) = \int_{\mathbb{R}^d} \frac{\rho(x+y)-\rho(y)-y\cdot\nabla_x\rho(x)}{|y|^{\alpha+d}}dy.$$

Direct fully-implicit schemes are not AP

Assume we work on a bounded domain in space and velocity:

$$\frac{f^{n+1} - f^n}{\Delta t} + \varepsilon^{1-\alpha} v \cdot \nabla_x f^{n+1} = \varepsilon^{-\alpha} \nu (\rho^{n+1} M - f^{n+1}).$$

$$\widehat{f}^{n+1} = \frac{\nu}{\nu + i\varepsilon\lambda k \cdot v} \left(\lambda \widehat{\rho}^{n+1} M + (1-\lambda) \widehat{f}^n \right).$$

$$\lambda = \frac{\nu \Delta t / \varepsilon^\alpha}{1 + \nu \Delta t / \varepsilon^\alpha}.$$

$$\rho^{n+1} = \left\langle \frac{(1-\lambda)\nu + i\varepsilon\lambda k \cdot v}{\nu + i\varepsilon\lambda k \cdot v} \nu M \right\rangle^{-1} \left\langle \frac{(1-\lambda)\nu^2}{\nu + i\varepsilon\lambda k \cdot v} f^n \right\rangle.$$

At fixed Δt, the limit $\varepsilon \to 0$ gives, for $1 < \alpha < 2$:

$$\rho^{n+1} = \rho^n, \qquad f^{n+1} = \rho^{n+1} M.$$

So the "limit $\varepsilon \to 0$ then $\Delta t \to 0$" is not correct.

Large velocity effect: not captured

$$\Delta t = 10^{-3},\ \varepsilon = 10^{-6}$$

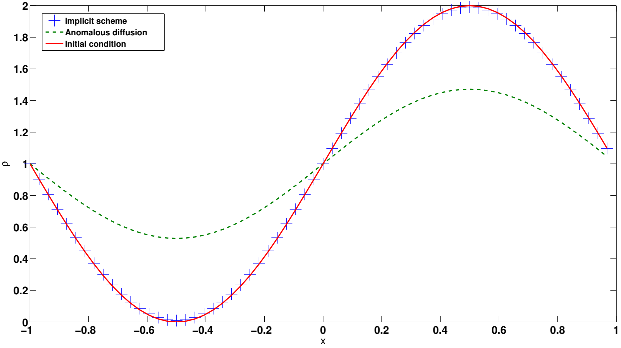


Figure: For $\Delta t = 10^{-3}$ the result given by the implicit scheme computed for $\varepsilon = 10^{-6}$ compared to the Euler scheme for the anomalous diffusion equation and the initial data.

Modified fully implicit scheme

- Even time-resolved implicit schemes do not work! The "limit $\Delta t \to 0$ then $\varepsilon \to 0$" is not correct any more.
- The effect of large or small velocities has not been taken into account.
- Perform a suitable change of variable before discretizing in velocity, on the following formulation of the scheme

$$\rho^{n+1} = \left[\left\langle \frac{(1-\lambda)\nu}{\nu + i\varepsilon\lambda k\cdot v} \nu M \right\rangle + \left\langle \frac{\varepsilon^2\lambda^2 (k\cdot v)^2}{\nu^2 + \varepsilon^2\lambda^2 (k\cdot v)^2} \nu M \right\rangle \right]^{-1} \left\langle \frac{(1-\lambda)\nu^2}{\nu + \varepsilon\lambda k\cdot v} f^n \right\rangle.$$

Take $w = \varepsilon\lambda v/\nu(v)$ in the red bracket only.

$$\rho^{n+1} = \left[\left\langle \frac{(1-\lambda)\nu}{\nu + i\varepsilon\lambda k\cdot v} \nu M \right\rangle + \text{"}\varepsilon^\alpha \lambda^\alpha D_\alpha |k|^\alpha\text{"} \right]^{-1} \left\langle \frac{(1-\lambda)\nu^2}{\nu + \varepsilon\lambda k\cdot v} f^n \right\rangle.$$

Since $1-\lambda \sim \varepsilon^\alpha/\Delta t$, when ε goes to 0, the limiting scheme is

$$\rho^{n+1} = \frac{\rho^n}{1 + \Delta t D_\alpha |k|^\alpha}.$$

Modified fully-implicit scheme: heavy-tail case

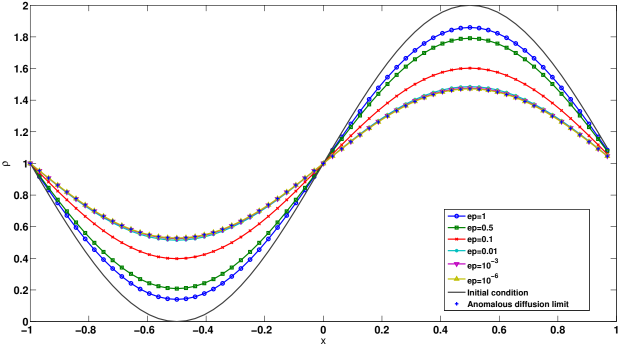


Figure: For $\Delta t = 10^{-3}$ the densities given by the modified implicit scheme for some ε and the anomalous diffusion limit. These densities converge to the anomalous diffusion solution when ε goes to zero.

Modified fully-implicit scheme: degenerate collision frequency

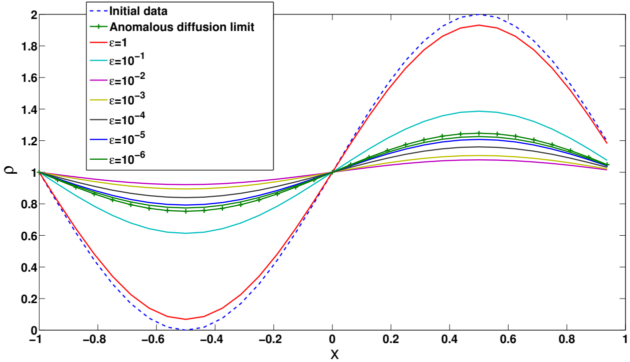


Figure: For $\Delta t = 10^{-3}$ the density profile converges to the anomalous diffusion solution when ε goes to zero.

Modified fully-implicit for $\varepsilon = 1$, heavy-tail case: order 1 in time

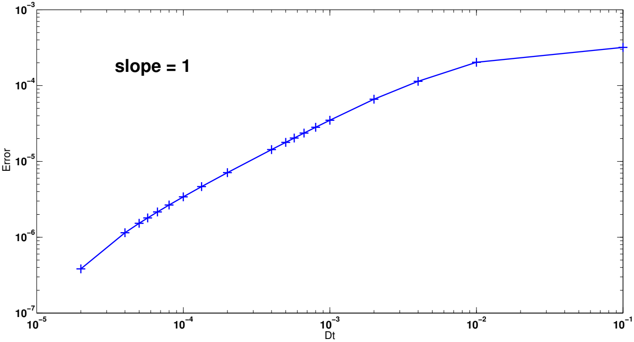


Figure: For $\varepsilon = 1$ the difference between the modified implicit scheme computed for $\Delta t = 10^{-5}$ and the same scheme computed for bigger Δt. It appears that the modified implicit scheme is of order 1 in Δt for $\varepsilon = 1$.

Modified fully-implicit scheme, heavy-tail case: behavior in ε

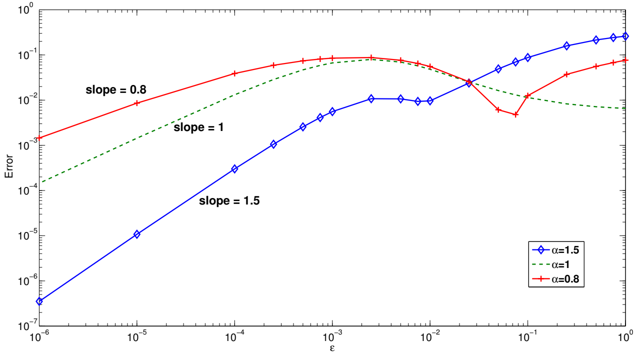


Figure: For $\Delta t = 10^{-3}$ and some values of α, the difference between the Euler scheme for anomalous diffusion and the modified implicit scheme computed for a range of ε. The convergence to the anomalous diffusion solution arises with speed α.

Slow convergence in the case of degenerate collision frequency: $\varepsilon^{d/(d+1+\beta)}$

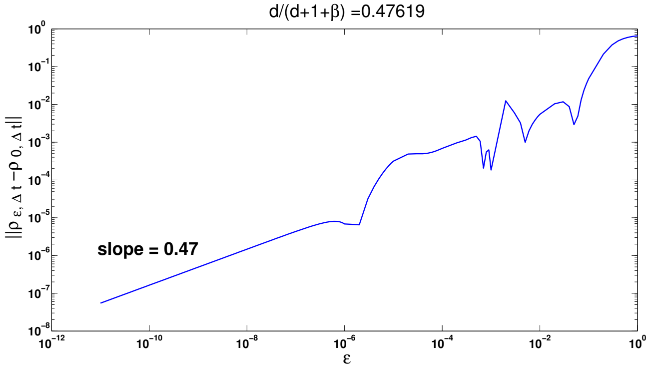


Figure: For $\Delta t = 10^{-2}$, $\beta = 0.1$. The convergence to the anomalous diffusion solution arises with speed $\varepsilon^{d/(d+1+\beta)}$.

Non uniform accuracy

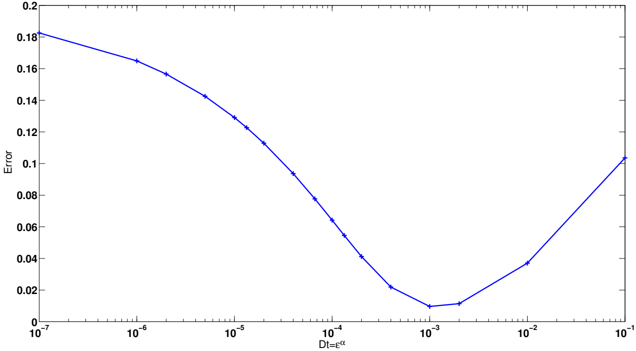


Figure: The error between the densities computed with the modified implicit scheme for $\Delta t = \varepsilon^{\alpha}$ and the density given by an implicit Euler scheme for the anomalous diffusion equation. This error does not converge to 0 for small Δt, illustrating the lack of uniformity of the implicit scheme.

Drawbacks of the fully-implicit scheme

- Inversion of transport operators may be expensive in case of non periodic boundary conditions for instance.
- Goal: construct AP schemes with completely explicit schemes. Tool: combine the above approach with suitable micro/macro scheme as done in [ML, CRAS 2010].

Usual micr/macro approach

- the usual micro/macro approach is based on the decomposition : $f = \rho M + g, \langle g \rangle = 0.$

$$
\begin{aligned}
&\partial_t \rho + \varepsilon^{1-\alpha} \langle v \cdot \nabla_x g \rangle = 0, \\
&\partial_t g + \varepsilon^{1-\alpha} v \cdot \nabla_x \rho M + \varepsilon^{1-\alpha} \left(v \cdot \nabla_x g - \langle v \cdot \nabla_x g \rangle M(v) \right) = \\
&\qquad\qquad -\frac{1}{\varepsilon^\alpha} \nu(v) \left(g - \frac{\langle \nu(v) g \rangle M}{\langle \nu(v) M(v) \rangle} \right).
\end{aligned}
$$

$$
\left\{
\begin{aligned}
\frac{\rho^{n+1} - \rho^n}{\Delta t} &+ \quad \varepsilon^{1-\alpha} \left\langle v \cdot \nabla_x g^{n+1} \right\rangle = 0 \\
\frac{g^{n+1} - g^n}{\Delta t} &+ \quad \varepsilon^{1-\alpha} v \cdot \nabla_x \rho^n M(v) + \varepsilon^{1-\alpha} \left(v \cdot \nabla_x g^n - \langle v \cdot \nabla_x g^n \rangle M(v) \right) \\
&= -\frac{1}{\varepsilon^\alpha} \nu(v) \left(g^{n+1} - \frac{\left\langle \nu(v) g^{n+1} \right\rangle}{\langle \nu(v) M(v) \rangle} M(v) \right),
\end{aligned}
\right.
$$

A suitable micro/macro scheme

- The strategy: keep the second equation explicit and replace the first by

$$\frac{\overline{\rho}^{n+1}-\overline{\rho}^{n}}{\Delta t}+\varepsilon^{1-\alpha}\langle v\cdot\nabla_x \tilde{f}^{n+1}\rangle=0$$

$$\tilde{f}^{n+1}=(\nu I+\varepsilon\lambda v\nabla_x)^{-1}(\lambda\nu\rho^{n+1}M)+(1-\lambda)(\nu f^n-\varepsilon\lambda v\nabla_x f^n).$$

- The resulting scheme

$$\frac{\overline{\rho}^{n+1}-\overline{\rho}^{n}}{\Delta t}+\varepsilon^{1-\alpha}\left\langle v\cdot\nabla_x(\nu I+\varepsilon\lambda v\nabla_x)^{-1}\lambda\nu M\rangle\rho^{n+1}\right\rangle$$
$$+\varepsilon^{1-\alpha}\langle(1-\lambda)\nu v\cdot\nabla_x(f^n-\varepsilon\lambda v\cdot\nabla_x f^n)\rangle=0.$$

- The change of variable in the first integral: $w=\varepsilon\lambda v$.

$$\frac{\overline{\rho}^{n+1}-\overline{\rho}^{n}}{\Delta t}+\lambda^{\alpha}(-\Delta)^{\alpha/2}\rho^{n+1}+\left\langle\frac{\varepsilon}{\varepsilon^{\alpha}+\nu\Delta t}v\cdot\nabla_x g^n\right\rangle=0.$$

$$\frac{g^{n+1}-g^{n}}{\Delta t}+\varepsilon^{1-\alpha}v\cdot\nabla_x\rho^n M(v)+\varepsilon^{1-\alpha}(v\cdot\nabla_x g^n-\langle v\cdot\nabla_x g^n\rangle M(v))$$
$$=-\frac{1}{\varepsilon^{\alpha}}\nu(v)\left(g^{n+1}-\frac{\langle\nu(v)g^{n+1}\rangle}{\langle\nu(v)M(v)\rangle}M(v)\right).$$

Densities with the micro/macro scheme for different values of ε

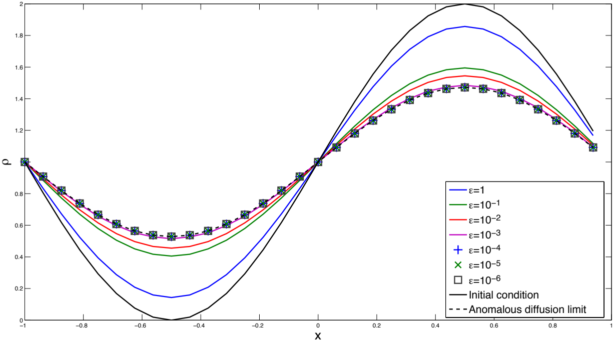


Figure: For $\Delta t = 10^{-2}$ the densities given by the modified micro-macro scheme for different values of ε and the anomalous diffusion limit.

Convergence in ε^{α} when $\varepsilon \to 0$.

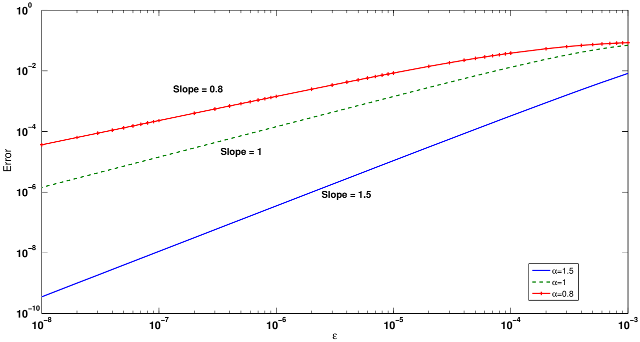


Figure: For $\Delta t = 10^{-3}$ the difference between the Euler scheme for anomalous diffusion and the modified micro-macro scheme computed for a range of ε.

Remarks on the micro/macro scheme

- The scheme is able to capture the right dynamics for $\varepsilon \sim 1$ and $\varepsilon << 1$.
- No inversion is needed for the transport operator. Transport terms are completely explicit.
- The scheme is of order one in time.
- The accuracy is not uniform.

Duhamel formulation and Anomalous diffusion

Goal: construct a scheme with a uniform accuracy: *order 1 in time uniformly in ε.*

We discretize in time: $t_n = n\Delta t$, $n = 0, ..., N$, and write

$$\widehat{\rho}(t_{n+1}, k) = \left\langle \exp\left(-\frac{\Delta t}{\varepsilon^\alpha}(1 + i\varepsilon k \cdot v)\right) \widehat{f}(t_n, k, v)\right\rangle + \int_0^{\frac{\Delta t}{\varepsilon^\alpha}} e^{-s}\langle e^{-i\varepsilon sk\cdot v} M(v)\rangle \widehat{\rho}(t^{n+1} - \varepsilon^\alpha s, k) ds.$$

Then we use a suitable quadrature to approximate the integral

$$\widehat{\rho}(t_{n+1} - \varepsilon^\alpha s) \sim a(s)\widehat{\rho}(t_n) + (1 - a(s))\widehat{\rho}(t_{n+1}), \qquad a(s) = \frac{\varepsilon^\alpha s}{\Delta t}, \quad 0 \leq a(s) \leq 1.$$

This quadrature of order 2. Local error in Δt^3.

The scheme is of order 2 for fixed $\varepsilon > 0$.

AP property of the Duhamel scheme

$$\widehat{\rho}^{n+1} = \exp\left(-\frac{\Delta t}{\varepsilon^\alpha}\right) A(\widehat{f_n}) + b\widehat{\rho}^n + c\widehat{\rho}^{n+1}$$

$$b = \int_0^{\frac{\Delta t}{\varepsilon^\alpha}} \frac{\varepsilon^\alpha s}{\Delta t} e^{-s} \langle e^{-i\varepsilon s k\cdot v} M(v)\rangle ds,$$

$$c = \int_0^{\frac{\Delta t}{\varepsilon^\alpha}} \left(1 - \frac{\varepsilon^\alpha s}{\Delta t}\right) e^{-s} \langle e^{-i\varepsilon s k\cdot v} M(v)\rangle ds.$$

We write

$$b = \int_0^{\frac{\Delta t}{\varepsilon^\alpha}} \frac{\varepsilon^\alpha s}{\Delta t} e^{-s} \langle (e^{-i\varepsilon s k\cdot v} - 1) M(v)\rangle ds + \int_0^{\frac{\Delta t}{\varepsilon^\alpha}} \frac{\varepsilon^\alpha s}{\Delta t} e^{-s} ds$$

and perform the change of variable $w = \varepsilon v$ on the first part before discretizing it in velocity.

Theorem

- *The scheme is of order 2 for any fixed $\varepsilon > 0$.*
- *The scheme is AP. The limiting scheme is of order 1 but can be modified to be of order 2 in the limit.*
- *The scheme is of order 1 uniformly in ε.*

Heavy-tail case: AP property

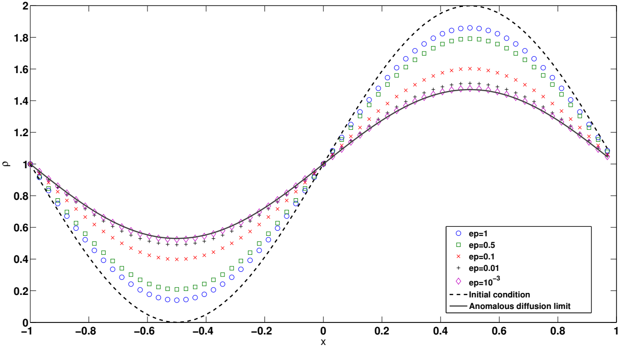


Figure: For $\Delta t = 10^{-3}$ the densities given by Duhamel based scheme for a decreasing range of ε and the anomalous diffusion limit. We observe that these densities converge to the anomalous diffusion solution when ε goes to zero.

convergence to the limit model when $\varepsilon \to 0$

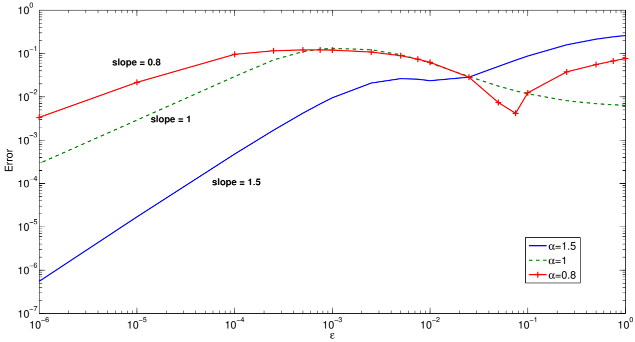
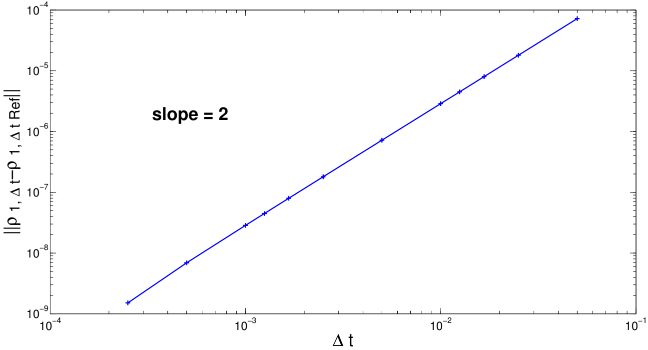
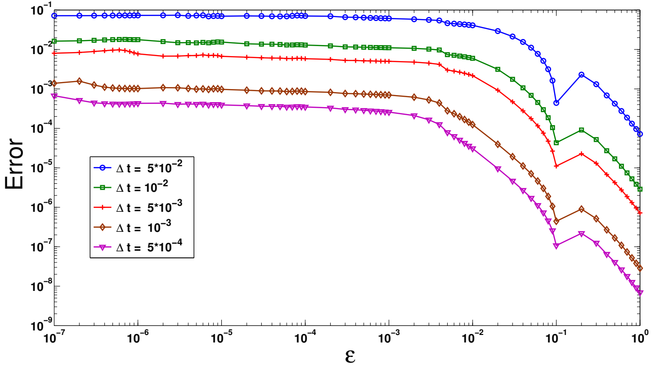


Figure: For $\Delta t = 10^{-3}$ and different cases of α, the difference between the Euler scheme for anomalous diffusion and the Duhamel formulation based scheme computed for a range of ε. We observe that the convergence to the anomalous diffusion solution arise with a speed α in ε.

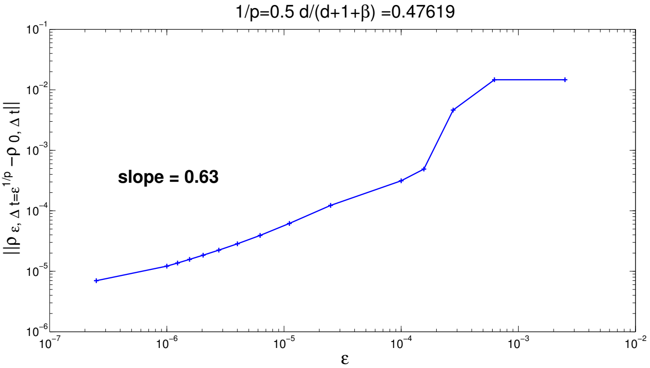
Duhamel method is of order 2 for fixed ε: $\beta = 1$



Duhamel method is of order 1 uniformly in ε: $\beta = 1$ and degenerate collision frequency



Uniform order is at least 1 : $\beta = 0.1$



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