Fractional derivatives, boundary value problems and heavy particles in a viscous fluid

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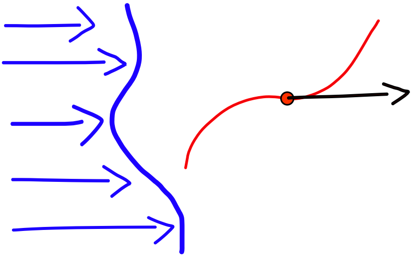
The Maxey-Riley equation

(M&R 1983)



$$\frac{d}{dt}\bar{x} = \bar{w} + \bar{u}(\bar{x}, t),$$

$$\frac{d}{dt}\bar{w} + \alpha\bar{w} + \gamma\frac{d}{dt}\int_0^t \frac{\bar{w}(s)}{\sqrt{t-s}}ds = \nabla\bar{u}\,\bar{w} + r\left(\frac{D\bar{u}}{Dt} - \bar{g}\right)$$

where $\bar{u}$ is a given fluid velocity, $\bar{w}$ is velocity of particle relative to fluid and $\bar{x}$ is location of the particle

$$r = \left(\frac{3R}{2} - 1\right),\ \alpha = \mu,\ \gamma = \kappa\mu^{1/2}$$

$$R = \frac{2\rho_f}{\rho_f + \rho_p},\ \mu = \frac{R}{St},\ \kappa = \sqrt{\frac{9R}{2\pi}},\ St = \frac{2}{9}\left(\frac{a}{L}\right)^2 Re$$

Faxén corrections may also be added.

Why are MR equations hard?

- Memory cost increases with time
- Computational cost increases with time
- Singular integrals
- Not a dynamical system

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All of this is really due to that nonlocal term

Known results

- (F&H 2015; L, F&H 2015) Local and global existence-uniqueness of mild solutions
- Proof is involved and delicate. Does not lead to a numerical method
- Long time behaviour
- Numerical schemes: Daitche (2015, 2013)
- Does history matter?

What can we say?

V,GP&G 2018; GP,V&G 2018

- A simpler proof of global existence using standard arguments
- ......once we reformulate the problem!
- Smoothness of solutions
- A new efficient numerical method to simulate the trajectory of the particle

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Main message

Think of the Maxey-Riley equation as a nonlinear boundary condition to the heat equation

Fractional derivatives

What makes MR hard? $\equiv$ What is a half-derivative?

$$\frac{d^{1/2}}{dt^{1/2}}y = \frac{d}{dt}\int_0^t \frac{y(s)}{\sqrt{t-s}}ds = \int_0^t \frac{\dot{y}(s)}{\sqrt{t-s}}ds + \frac{y(0)}{\sqrt{t}}$$

$$\frac{d^{1/2}}{dt^{1/2}}\frac{d^{1/2}}{dt^{1/2}}y = \frac{d}{dt}y$$

- Above is called Riemann-Liouville half-derivative. We'll stick to this.
- Many other definitions of fractional derivatives: Caputo, Atangana-Baleanu, Riesz, Hadamard, Marchaud, Grünwald-Letnikov and many others
- $$\left(\frac{d}{dt}\right)^{\alpha} y = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}|k|^{\alpha}\hat{y}(k)dk$$
- Fractional derivatives: Podlubny (1998). Equivalence of fractional Laplacians: Kwaśnicki (2017).

$$\frac{d^{1/2}}{dt^{1/2}}\frac{d^{1/2}}{dt^{1/2}}q = \frac{d}{dt}q$$

Formally replace

$$\frac{d^{1/2}}{dt^{1/2}} \to \frac{d}{dx}$$

to obtain

$$\frac{d^2}{dx^2}q = \frac{d}{dt}q$$

Does the 1/2 derivative have anything to do with the heat equation?

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Does the 1/2 derivative have anything to do with the heat equation?

$$q_t = q_{xx}, \quad x > 0, \ 0 < t < T,$$
$$q(x,0) = 0, \quad x > 0, t = 0, \quad q(0,t) = y(t), \quad 0 \le t \le T$$

Then

$$q_x(0,t) = \frac{d^{1/2}}{dt^{1/2}}y = \int_0^t \frac{\dot{y}(s)}{\sqrt{t-s}}ds + \frac{y(0)}{\sqrt{t}}$$

Dirichlet→Neumann map

Can be shown using UTM starting from the global relation

UTM: Dirichlet to Neumann map

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Global relation

$$e^{k^2 T}\hat{q}(k,T) = ik\tilde{f}_0(k,0,T) + \tilde{f}_1(k,0,T), \quad k \in \mathbb{C}^-$$

$$\hat{q}(k,T) = \int_0^\infty e^{-ikx} q(x,T)dx, \quad \tilde{f}_j(k,X,\tau) = \int_0^\tau e^{k^2 s}\partial_x^j q(X,s)ds$$

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- Multiply by $ike^{-ik^2 t}$ and integrate over $\partial D^- = \{k \in \mathbb{C}^- \mid \operatorname{Re} k^2 = 0\}$
- Left-hand side drops out by Jordan's lemma
- Right most term $k^2 \to il$, $l \in \mathbb{R}$ and apply Fourier inversion theorem
- Integrate-by-parts first term on right and then apply Fubini's theorem

Model equation

MR equation

$$\frac{d}{dt}\bar{x} = \bar{w} + \bar{u}(\bar{x}, t),$$

$$\frac{d}{dt}\bar{w} + \alpha\bar{w} + \gamma\frac{d}{dt}\int_0^t \frac{\bar{w}(s)}{\sqrt{t-s}}ds = \bar{F}(\bar{w}, \bar{x}, t)$$

Focus attention on the velocity equation and replace nonlinearity

$$\frac{d\bar{y}}{dt} + \alpha\bar{y} + \gamma\frac{d^{1/2}}{dt^{1/2}}\bar{y} = \bar{F}(\bar{y})$$

Linear version

$$\frac{d\bar{y}}{dt} + \alpha\bar{y} + \gamma\frac{d^{1/2}}{dt^{1/2}}\bar{y} = \bar{F}(t)$$

Q Can we solve this equation?

- F&H (2015) invert the d/dt and iterate over space of continuous functions

Model equation

(scalar linear) Model MR $\to$ Heat equation

$y(t) \to q(0,t)$

$$\begin{aligned}
q_t &= q_{xx}, \quad x > 0,\ 0 < t < T, \\
q(x,0) &= 0, \quad x > 0, t = 0, \\
\frac{d}{dt} q(0,t) + \alpha q(0,t) - \gamma q_x(0,t) &= F(t), \quad 0 \le t \le T, \\
\lim_{t \to 0} q(0,t) &= y_0
\end{aligned}$$

Q Can we solve this boundary-value problem?

A Yes! Using UTM

Model equation

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\end{aligned}
$$

Q Can we solve this boundary-value problem?
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Q What does 'solve' mean?

Nonlinear model MR

Local existence

Scalar model MR $\to$ mild form

$$\frac{dy}{dt} + \alpha y + \gamma \frac{d^{1/2}}{dt^{1/2}} y = F(y) \quad \longrightarrow \quad y(t) = \varphi(t) y_0 + \int_0^t \varphi(t-s) F(y(s)) ds$$

and Picard iterates converge in $C[0, T]$ for F Lipschitz

Nonlinear model MR

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$$\frac{dy}{dt} + \alpha y + \gamma \frac{d^{1/2}}{dt^{1/2}} y = 0, \quad y(0) = y_0$$

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$$\frac{dy}{dt} + \alpha y + \gamma \frac{d^{1/2}}{dt^{1/2}} y = 0, \quad y(0) = y_0$$

in the sense

$$\begin{aligned} q_t = q_{xx}, \quad x > 0,\ 0 < t < T, \\ q(x,0) = 0, \quad x > 0, t = 0, \\ \frac{d}{dt} q(0,t) + \alpha q(0,t) - \gamma q_x(0,t) = 0, \quad 0 \le t \le T, \\ \lim_{t \to 0} q(0,t) = y_0 \end{aligned}$$

has a solution and $\lim_{x \to 0} q(x,t) = \varphi(t)$

Nonlinear model MR

Local existence

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$$\frac{dy}{dt} + \alpha y + \gamma \frac{d^{1/2}}{dt^{1/2}} y = F(y) \quad \longrightarrow \quad y(t) = \varphi(t) y_0 + \int_0^t \varphi(t-s) F(y(s)) ds$$

and Picard iterates converge in $C[0,T]$ for F Lipschitz where

$$\varphi(t) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{k e^{-k^2 t}}{\alpha - k^2 + ik\gamma} dk$$

Nonlinear model MR

Local existence

Scalar model MR $\rightarrow$ mild form

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and Picard iterates converge in $C[0,T]$ for F Lipschitz where

$$\varphi(t) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{k e^{-k^2 t}}{\alpha - k^2 + ik\gamma} dk$$

- $\varphi(0) = 1$, $\varphi'(t) < 0$ for $t > 0$ and $\varphi(t) \to 0$ as $t \to \infty$
- $\varphi(t)$ is bounded, $1/2-$Hölder continuous at $t = 0$ and smooth for all $t > 0$
- If F is differentiable $\Rightarrow$ strong solution for $t > 0$
- Grönwall's inequality implies uniqueness

Nonlinear model MR

Global existence

Classical argument

$$\frac{dy}{dt} = F(y) \quad \longrightarrow \quad y(t) = y_0 + \int_0^t F(y(s))ds$$

Local existence in $C[0, T]$. Restart the iteration process using $y_0 = y(T)$

In our case $\varphi(t+s) \neq \varphi(t)\varphi(s)$. No semigroup property

$t \to t+s$ implies vector field at $t+s$ depends on solution up to time s

Not a dynamical system!

Nonlinear model MR

Global existence

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Not a dynamical system!

... But heat equation is!

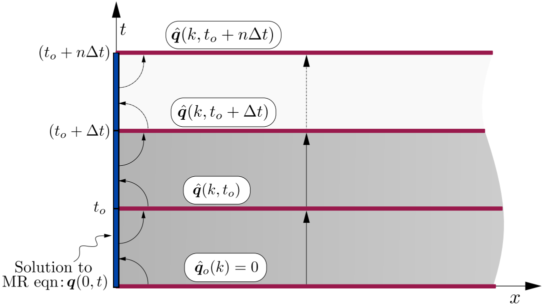
Linear model MR

Global existence

$$q_t = q_{xx}, \quad x > 0, t \in (t_0, t_0 + \Delta t),$$
$$\frac{d}{dt}q(0,t) + \alpha q(0,t) - \gamma q_x(0,t) = F(t), \quad t_0 \le t \le t_0 + \Delta t,$$
$$\lim_{t \to t_0} q(0,t) = y(t_0),$$
$$q(x, t_0) = q_{t_0}(x) \longleftarrow \text{ Now specified}$$

1) solve for Dirichlet condition in $[t_0, t_0 + \Delta t]$

2) find $q(x, t_0 + \Delta t)$ using Dirichlet boundary condition



Nonlinear model MR

Same idea works for nonlinear case

$$
\begin{aligned}
q_t &= q_{xx}, \quad x > 0, t \in (t_0, t_0 + \Delta t), \\
\frac{d}{dt} q(0,t) + \alpha q(0,t) - \gamma q_x(0,t) &= F(q(0,t)), \quad t_0 \le t \le t_0 + \Delta t, \\
\lim_{t \to t_0} q(0,t) &= y(t_0), \\
q(x, t_0) &= q_{t_0}(x) \longleftarrow \text{ Now specified}
\end{aligned}
$$

- Only require $\hat{q}(k, t_0)$ (no Fourier inversion required)
- If nonlinearity is uniformly Lipschitz $\Rightarrow$ Global existence (usual ODE argument)
- $y(t)$, $t \in [t_0, t_0 + \Delta t] \to \hat{q}(k, t_0 + \Delta t)$ is explicit

Nonlinear model MR

$$y(t) = \int_{-\infty}^{\infty} k e^{-k^2(t-t_0)} \hat{H}(k,t_0) dk + \int_{t_0}^{t} F(y(s))\varphi(t-s)ds, \quad t_0 < t < t_0 + \Delta t$$

$$\hat{H}(k,t_0) = e^{-k^2 \Delta t}\, \hat{H}(k, t_0 - \Delta t) - e^{-k^2 t_0} \int_{t_0-\Delta t}^{t_0} e^{k^2 s} y(s) ds$$
$$+ \frac{e^{-k^2 t_0}}{\alpha - k^2 + i\gamma k} \int_{t_0-\Delta t}^{t_0} e^{k^2 s} F(y(s)) ds$$

with

$$\hat{H}(k,0) = \frac{y(0)}{(\alpha - k^2 + ik\gamma)}$$

and

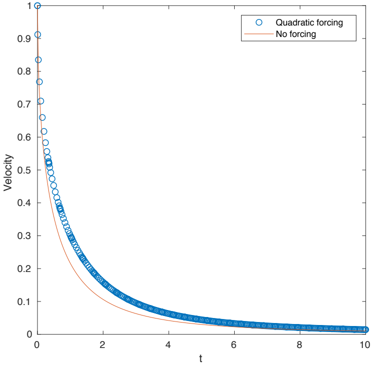
$$\varphi(t) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{k e^{-k^2 t}}{\alpha - k^2 + ik\gamma} dk$$

- Rewriting history along the way

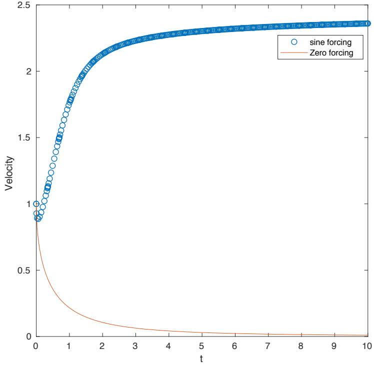
Numerical method

- Approximate $y(t)$ in Chebyshev polynomials over interval $[t_0, t_0 + \Delta t]$
- Use mapped Chebyshev polynomials for $\hat{H}(k, t_0)$
- Newton's method to solve for $y(t)$. Convergence follows from existence of local solution

$$\frac{d}{dt} y + y - \frac{d^{1/2}}{dt^{1/2}} y = F(y)$$



$F(y) = y^2$



$F(y) = -4\sin(y)$

Back to the MR equations

Component-wise

$$\frac{dx_i}{dt} = w_i + u_i(\bar{x}, t),$$
$$\frac{dw_i}{dt} + \alpha w_i + \gamma \frac{d^{1/2}}{dt^{1/2}} w_i = F_i(\bar{x}, \bar{w}, t)$$

- This leads to a system of model equations
- Linear equations are decoupled, solved using UTM
- Three heat equation BVPs (but effectively all are same)

Theorem

If $\bar{u}$ is sufficiently smooth, then for any initial condition the MR equations has a mild solution for all time $t > 0$

- Velocities are differentiable except possibly at $t = 0$ (when $w_i(0) \neq 0$)
- Fluid velocity $\bar{u}(\bar{x}, t)$ has three continuous uniformly bounded derivatives and partial derivatives are uniformly Lipschitz (same as F&H 2015)

Why stick to only half-derivatives?

Rational derivatives

$$\frac{d}{dt}y + \alpha y + \gamma \frac{d^{1/3}}{dt^{1/3}} y = 0, \quad y(0) = y_0$$

rewritten as

$$\begin{aligned} q_t &= -q_{xxx}, \quad x > 0,\ t \in (0,T), \\ q(x,0) &= 0, \quad x > 0, \\ \frac{d}{dt}q(0,t) + \alpha q(0,t) + \gamma q_x(0,t) &= 0, \quad t \in [0,T], \\ \lim_{t\to 0} q(0,t) &= y_0 \end{aligned}$$

since

$$\frac{d^{1/3}}{dt^{1/3}} y = \int_0^t \frac{\dot{y}(s)}{(t-s)^{1/3}} ds + \frac{y_0}{t^{1/3}} = q_x(0,t) = DN[q(0,t)]$$

where $DN[f]$ is the Dirichlet to Neumann map for the third order PDE.

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where $DN[f]$ is the Dirichlet to Neumann map for the third order PDE.

also

$$\frac{d^{2/3}}{dt^{2/3}} y = q_{xx}(0,t)$$

Rational derivatives

a general recipe

$$q_t = \partial_x^n q, \quad x > 0,\ 0 < t < T$$
$$q(0,t) = y(t), \quad t \in [0,T]$$
$$\partial_x^m q(0,t) = \frac{d^{m/n}}{dt^{m/n}} y$$

$$\mathcal{L}q = \partial_x^n q, \quad q(x,t) : \mathbb{R}^+ \times \Omega \to \mathbb{R},\ \Omega \subset \mathbb{R}^n$$
$$q(0,t) = y(t), \quad t \in \Omega$$
$$\partial_x^m q(0,t) = \mathcal{L}^{m/n} y$$

e.g. $\mathcal{L}$ could be negative Laplacian or even wave operator. Compare elliptic extension due to Cafarelli and Sylvestre (2007)

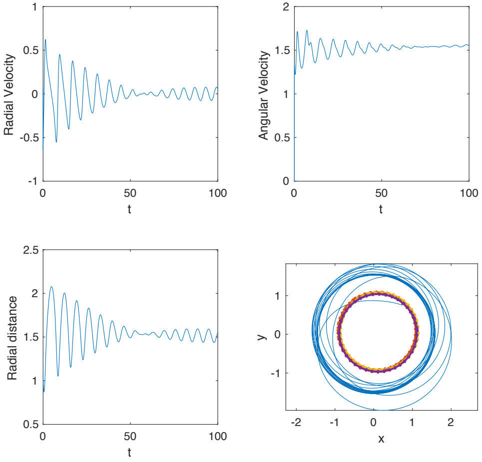
$$\Delta_t \tilde{u} + \frac{1-\alpha}{x}\partial_x \tilde{u} + \tilde{u}_{xx} = 0,$$
$$\tilde{u}(t,0) = u(t).$$

Then

$$(-\Delta_t)^{\alpha/2} u = c \lim_{x\to 0} \frac{\tilde{u}(x,t) - u(t)}{x^\alpha}.$$

Conclusions

- A new way to consider rational derivatives
- Simpler wellposedness proof for MR equations
- Efficient numerical method for MR equations with fixed memory cost



Particle amongst three point-vortices

What remains?

- Explicit time integrators
- Integration with DNS of Navier-Stokes
- ...Does history matter?