A regularised particle method for linear and nonlinear diffusion

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Contents

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Background

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- $U_m \colon [0,\infty) \to \mathbb{R}$, $m \geq 1$, is a density of **internal** energy (diffusion),

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  For simplicity, V and W belong to $C^2(\mathbb{R}^d)$ and are bounded from below.

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$$\int_0^T \int_{\mathbb{R}^d} \left(\partial_t \psi(t,x) + \langle \nabla \psi(t,x), \nabla \phi(t,x) \rangle\right) \, \mathrm{d}\mu_t(x) \, \mathrm{d}t = 0.$$

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and equip it with the 2-**Wasserstein** distance

$$W_2(\mu,\nu) = \min_{\pi \in \Pi(\mu,\nu)} \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |x-y|^2 \,\mathrm{d}\pi(x,y) \right)^{1/2} \quad \text{for all } \mu,\nu \in \mathcal{P}_2(\mathbb{R}^d),$$

where $\Pi(\mu,\nu)$ is the set of probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with first marginal μ and second marginal ν.

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Under suitable regularity conditions on V, W and μ, we can show that

$$(\mathcal{E}^m)'_\mu(x) = U'_m(\mu(x)) + V(x) + W * \mu(x) \quad \text{for all } x \in \mathbb{R}^d.$$

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Thus (1) becomes

$$\mu'(t) = -\nabla_{W_2}\mathcal{E}^m(\mu(t)) \quad \text{for a.e. } t \in [0, T],$$

and so our continuity equation is a **gradient flow** for $\mathcal{E}^m$.

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$$\mu^0 \simeq \mu_N^0 = \sum_{i=1}^N m_i \delta_{x_i^0}, \qquad m_i > 0, \quad (x_i^0)_{i\in\{1,\dots,N\}} \subset \mathbb{R}^d.$$

Then, under suitable conditions on V and W and if $\mu_N^0 \in \overline{D(\mathcal{E}^0)}$, the solution μ_N to (2) with initial datum μ_N^0 stays a combination of point masses, i.e.,

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We may define a particle method simply by solving the ODE system

$$\dot{x}_i(t) = -\nabla V(x_i(t)) + \sum_{j=1}^N m_j W(x_i(t) - x_j(t)).$$

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The convergence of this particle method and other properties of (2) have been widely studied:

- Laurent (2007); Bertozzi–Laurent–Rosado (2011);
- Carrillo–Di Francesco–Figalli–Laurent–Slepčev (2011);
- Carrillo–Choi–Hauray (2014);
- Jabin (2014),...

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For most of this talk we only focus on the **diffusion** part, i.e.,

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Goal. Derive a **deterministic** particle method approximating (3) that respects the underlying **gradient-flow** structure and which works naturally in **higher dimensions**.

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- Solve the gradient flow for $\mathcal{F}_\varepsilon^m$:

$$\mu_t' = -\nabla_{W_2}\mathcal{F}_\varepsilon^m(\mu_t). \tag{4}$$

We have

$$(\mathcal{F}_\varepsilon^m)_\mu' = \varphi_\varepsilon * (\mu F_m' \circ (\varphi_\varepsilon * \mu)) + F_m \circ (\varphi_\varepsilon * \mu),$$

and so (4) becomes

$$\mu_t' = \operatorname{div}\Big(\mu_t \nabla\varphi_\varepsilon * (\mu_t F_m' \circ (\varphi_\varepsilon * \mu_t)) + \mu_t(\nabla\varphi_\varepsilon * \mu_t) F_m' \circ (\varphi_\varepsilon * \mu_t)\Big).$$

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The case $m = 2$ is very particular. Indeed,

$$F_2'(s) = 1, \qquad \mu_t' = 2 \operatorname{div}(\mu_t \nabla \varphi_\varepsilon * \mu_t),$$

which is an interaction equation with kernel $2\varphi_\varepsilon$.

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$$\dot{x}_i = -\sum_{j=1}^N m_j \nabla \varphi_\varepsilon(x_i - x_j) \left(F_m' \left(\sum_{k=1}^N m_k \varphi_\varepsilon(x_j - x_k) \right) + F_m' \left(\sum_{k=1}^N m_k \varphi_\varepsilon(x_i - x_k) \right) \right).$$

The case $m = 2$ is very particular. Indeed,

$$F_2'(s) = 1, \qquad \mu_t' = 2 \operatorname{div}(\mu_t \nabla \varphi_\varepsilon * \mu_t),$$

which is an interaction equation with kernel $2\varphi_\varepsilon$. This is the same equation as Lions–Mas-Gallic studied; our method is therefore a generalisation of theirs to any porous medium equation.

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- **Convergence of gradient flows.** When $m = 2$ and under suitable regularity assumptions on the regularised gradient flows $(\mu_\varepsilon)_\varepsilon$, the gradient flow for $\mathcal{F}_\varepsilon^m$ converges to that for $\mathcal{F}^m$ in the Sandier–Serfaty sense.

Results

Assumptions on the mollifier. Let $\zeta \in C^2(\mathbb{R}^d \times [0, +\infty))$ be even, $\|\zeta\|_{L^1(\mathbb{R}^d)} = 1$, and assume there exist $C_\zeta, C'_\zeta > 0$, $q > d+1$, and $q' > d$ such that

$$\zeta(x) \leq C_\zeta |x|^{-q}, \quad |\nabla \zeta(x)| \leq C'_\zeta |x|^{-q'} \quad \text{for all } x \in \mathbb{R}^d.$$

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Theorem (Serfaty, 2011). Let $m \ge 2$. Suppose that, for all $\varepsilon > 0$, μ_ε is a gradient flow for $\mathcal{F}^m_\varepsilon$ with well-prepared initial data, i.e.,

$$\mu_\varepsilon(0) \rightharpoonup \mu_0 \text{ narrowly}, \quad \lim_{\varepsilon\to 0} \mathcal{F}^m_\varepsilon(\mu_\varepsilon(0)) = \mathcal{F}^m(\mu(0)), \quad \mu_0 \in \mathcal{P}_2(\mathbb{R}^d).$$

Suppose further that there exists a curve $\mu\colon [0,T] \to \mathcal{P}_2(\mathbb{R}^d)$ such that, for almost every $t \in [0,T]$, $\mu_\varepsilon(t) \rightharpoonup \mu(t)$ narrowly and

(1) $\liminf_{\varepsilon\to 0} \int_0^t |\mu'_\varepsilon|(s)^2 \, \mathrm{d}s \ge \int_0^t |\mu'|(s)^2 \, \mathrm{d}s$,

(2) $\liminf_{\varepsilon\to 0} \mathcal{F}^m_\varepsilon(\mu_\varepsilon(t)) \ge \mathcal{F}^m(\mu(t))$,

(3) $\liminf_{\varepsilon\to 0} \int_0^t \left\| \nabla (\mathcal{F}^m_\varepsilon)'_{\mu_\varepsilon(s)} \right\|^2_{L^2(\mu_\varepsilon(s);\mathbb{R}^d)} \mathrm{d}s \ge \int_0^t \left\| \nabla (\mathcal{F}^m)'_{\mu(s)} \right\|^2_{L^2(\mu(s);\mathbb{R}^d)} \mathrm{d}s$.

Then μ is a gradient flow for $\mathcal{F}^m$.

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  That is the tough one: we need some **extra regularity** assumptions on the regularised gradient flows $(\mu_\varepsilon)_\varepsilon$.

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where $p_\varepsilon := \mu F_m' \circ (\varphi_\varepsilon * \mu)$. Note

$$\|\mu\|_{BV_\varepsilon^m} \geq \left\| \nabla (\mathcal{F}_\varepsilon^m)_\mu' \right\|_{L^1(\mu;\mathbb{R}^d)}.$$

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Theorem (Carrillo–Craig–P., 2017). Let $m \geq 2$, and $\mu_\varepsilon\colon [0,T] \to \mathcal{P}_2(\mathbb{R}^d)$ be a gradient flow for $\mathcal{F}_\varepsilon^m$ for all $\varepsilon > 0$ with well-prepared initial data with respect to $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$. Furthermore, suppose that the following hold:

(1) $\sup_{\varepsilon>0} \int_0^T M_{m-1}(\mu_\varepsilon(t))\,\mathrm{d}t < \infty$,

(2) $\sup_{\varepsilon>0} \int_0^T \|\mu_\varepsilon(t)\|_{BV_\varepsilon^m}\,\mathrm{d}t < \infty$,

(3) $\begin{cases} \zeta_\varepsilon * \mu_\varepsilon(t) \to \mu(t) & \text{in } L^1([0,T]; L^m_{\mathrm{loc}}(\mathbb{R}^d)) \text{ as } \varepsilon \to 0, \\ \sup_{\varepsilon>0} \int_0^T \|\zeta_\varepsilon * \mu_\varepsilon(t)\|^m_{L^m(\mathbb{R}^d)}\,\mathrm{d}t < \infty. \end{cases}$

Then $\mu_\varepsilon(t) \rightharpoonup \mu(t)$ narrowly for almost every $t \in [0,T]$ for some $\mu\colon [0,T] \to \mathcal{P}_2(\mathbb{R}^d)$, and μ is the gradient flow for $\mathcal{F}^m$ with initial datum μ_0.

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Numerical simulations

We now reintroduce the potentials V and W. Recall that our particle method is based on the ODE system

$$\dot{x}_i = -\sum_{j=1}^{N} m_j \nabla \varphi_\varepsilon(x_i - x_j) \left(F_m' \left(\sum_{k=1}^{N} m_k \varphi_\varepsilon(x_j - x_k) \right) + F_m' \left(\sum_{k=1}^{N} m_k \varphi_\varepsilon(x_i - x_k) \right) \right) - \nabla V(x_i) - \sum_{j=1}^{N} m_j \nabla W(x_i - x_j).$$

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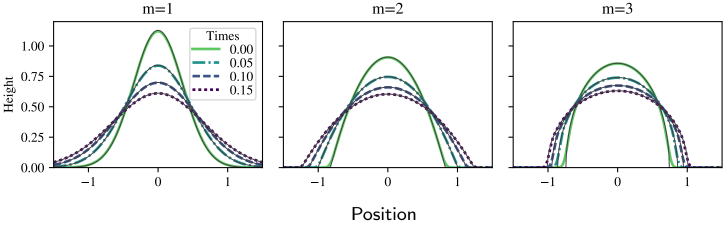
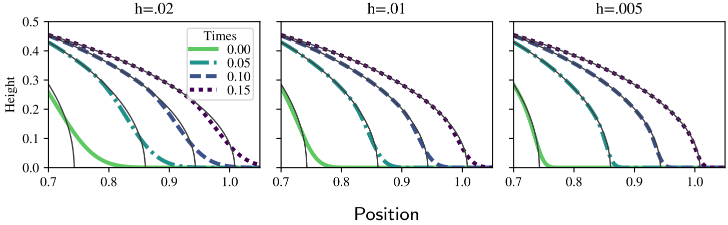
To visualise numerically our particle solution $\mu_{\varepsilon(h)}$, we convolve it with the mollifier ζ_ε; i.e., we plot $\tilde{\mu}_{\varepsilon(h)} = \zeta_\varepsilon * \mu_{\varepsilon(h)}$.

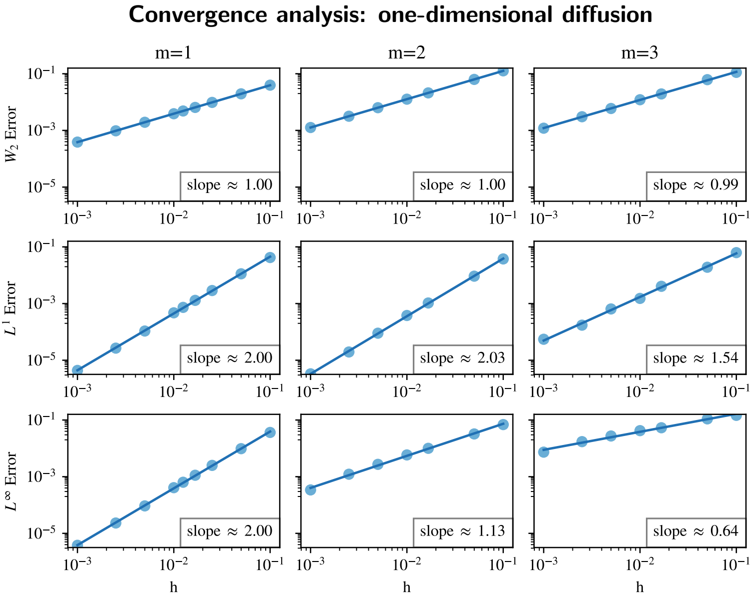
One-dimensional heat and porous medium equations: fundamental solutions

Exact vs numerical solution, $h = 0.02$, varying m

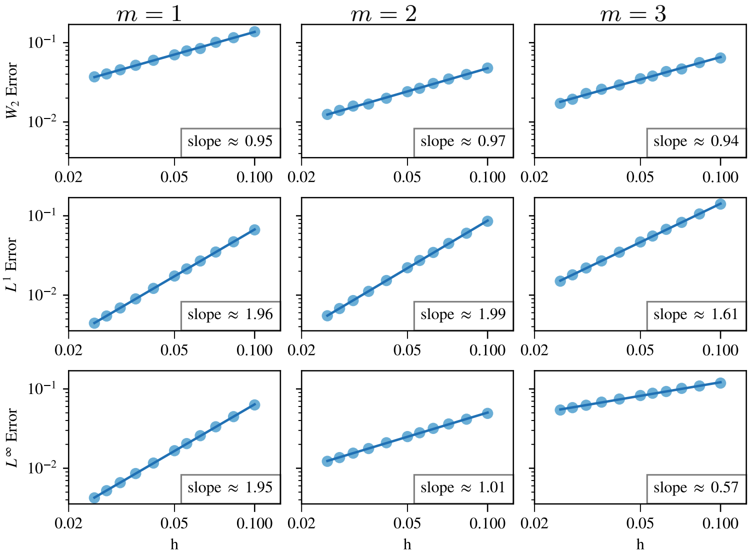


Exact vs numerical solution, varying h, $m = 3$

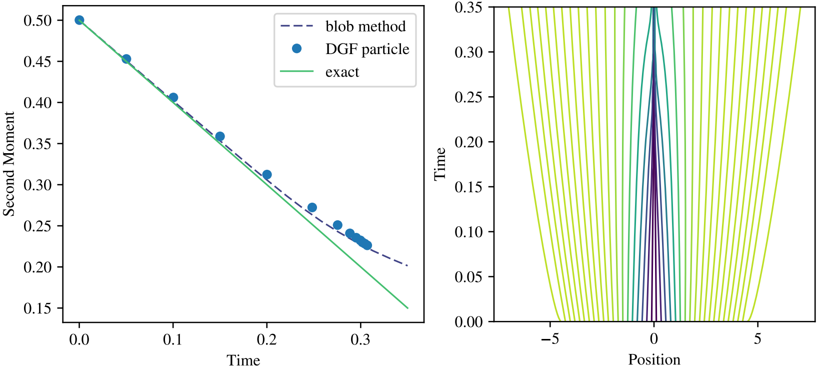



Convergence analysis: one-dimensional diffusion
m=1
m=2
m=3
W_2 Error
L^1 Error
L^∞ Error
slope ≈ 1.00
slope ≈ 1.00
slope ≈ 0.99
slope ≈ 2.00
slope ≈ 2.03
slope ≈ 1.54
slope ≈ 2.00
slope ≈ 1.13
slope ≈ 0.64
h
h
h

Convergence analysis: two-dimensional diffusion



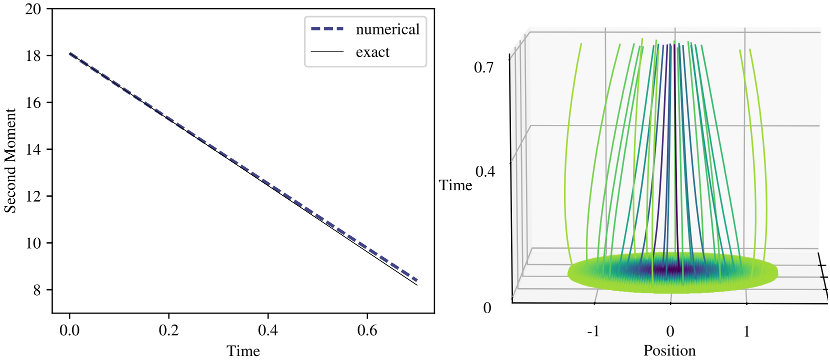
Modified one-dimensional Keller–Segel equation: blow-up with $\chi = 1.5$, $h = 0.009$



$$F_m(s) = F_1(s) = \log s, \quad W(x) = 2\chi \log |x|, \quad V(x) = 0.$$

(DGF: see Carrillo–Huang–P.–Wolansky (2017).)

Two-dimensional Keller–Segel equation: blow-up with supercritical mass 9π, $h = 0.03$



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- Can the semiconvexity estimate of $\mathcal{F}_\varepsilon^m$ be improved so that it does not degenerate as $\varepsilon \to 0$?

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THANK YOU!