Numerical Analysis of Some Singular PDEs with Logarithmic Nonlinearity

Li-Lian Wang

Division of Mathematical Sciences
School of Physical and Mathematical Sciences
Nanyang Technological University, Singapore
Email: lilian@ntu.edu.sg



Based on joint works with Jingye Yan (Jiangsu U.) & Boya Zhou (HuazhongUST)

Numerical Methods for Fractional-Derivative Problems, Beijing CSRC, 12/08/2022

Outline

- Examples and Motivations
- Existing Results: Theory & Numerics
- Direct Linearised CN Scheme
- Positive and Ground-State Solutions
- Numerical Results

Some PDEs with Logarithmic Nonlinearity¹

Heat equation with a logarithmic nonlinearity (Log-Heat)

$$u_t - \Delta u = \lambda u \ln |u| := \lambda f(u), \quad \lambda \neq 0, \quad \lambda \in \mathbb{R}$$

Logarithmic Schrödinger equation (LogSE)

$$iu_t + \Delta u = \lambda u \ln |u|$$

or LogSE with a potential V (e.g., $V = |x|^2$): $\Delta + V \rightarrow \Delta$.

¹Applications: nonlinear wave, quantum mechanics & optics; nuclear physical; superfluids & Bose-Einstein condensation, ... (cf. Białynicki-Birula & J. Mycielski, 1975)

Some PDEs with Logarithmic Nonlinearity¹

Heat equation with a logarithmic nonlinearity (Log-Heat)

$$u_t - \Delta u = \lambda u \ln |u| := \lambda f(u), \quad \lambda \neq 0, \quad \lambda \in \mathbb{R}$$

Logarithmic Schrödinger equation (LogSE)

$$iu_t + \Delta u = \lambda u \ln |u|$$

or LogSE with a potential
$$V$$
 (e.g., $V = |x|^2$): $\Delta + V \rightarrow \Delta$.

Logarithmic Klein-Gordon equation (LogKGE)

$$u_{tt} - \Delta u + u = \lambda u \ln |u|$$

¹Applications: nonlinear wave, quantum mechanics & optics; nuclear physical; superfluids & Bose-Einstein condensation, ... (cf. Białynicki-Birula & J. Mycielski, 1975)

• Cahn-Hilliard equation with logarithmic Flory-Huggins potential²

$$u_t = \Delta(-\Delta u + f(u)) \text{ with } f(u) = F'(u) = \frac{\theta_0}{2} \ln \frac{1+u}{1-u} - \theta_1 u,$$

and
$$F(u) = \frac{\theta_0}{2} \left((1+u) \ln(1+u) + (1-u) \ln(1-u) \right) - \frac{\theta_1}{2} u^2.$$

 $^{^2}$ If $\|u_0\|_{\infty} < 1$, then $\|u\|_{\infty} < 1$, see Elliot-Garcke'94, Debussche-Detttori'95.

Cahn-Hilliard equation with logarithmic Flory-Huggins potential²

$$u_t = \Delta(-\Delta u + f(u)) \text{ with } f(u) = F'(u) = \frac{\theta_0}{2} \ln \frac{1+u}{1-u} - \theta_1 u,$$
 and
$$F(u) = \frac{\theta_0}{2} \left((1+u) \ln(1+u) + (1-u) \ln(1-u) \right) - \frac{\theta_1}{2} u^2.$$

- Wasserstein gradient flows
 - Poisson-Nernst-Planck (PNP) system: $(c_1, c_2 > 0)$

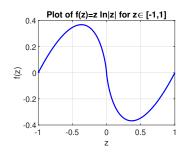
$$E[c_1, c_2, \phi] = \int_{\Omega} \left(c_1 (\ln c_1 - 1) + c_2 (\ln c_2 - 1) + \frac{1}{2} |\nabla \phi|^2 \right) dx$$

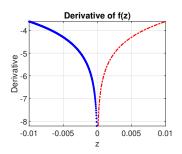
• Keller-Segel system with free energy: (0 < u < 1)

$$E[u,\phi] = \int_{\Omega} \left(u \ln u + (1-u) \ln(1-u) - u\phi + \frac{1}{2} |\nabla \phi|^2 + \frac{1}{2} \phi^2 \right) dx$$

 $^{^{2}\}text{If }\|u_{0}\|_{\infty}<1,$ then $\|u\|_{\infty}<1,$ see Elliot-Garcke'94, Debussche-Detttori'95.

Some Observations

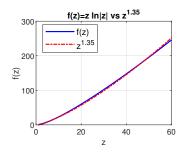


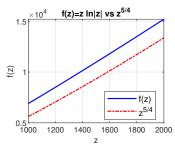


- Let $f(z) = z \ln |z|$. Then f(0) = 0 and f(-z) = -f(z).
- Non-differentiable at z = 0, as

$$f'(z) = 1 + \ln|z|, \quad z \neq 0$$

Growth of f(z) for z > 1





• The function $f(z) = z \ln |z|$ grows like

$$f(z) = |z|^p z, \quad 0$$

and $f(z) = o(z^{1+\epsilon})$ for $z \gg 1$.

6

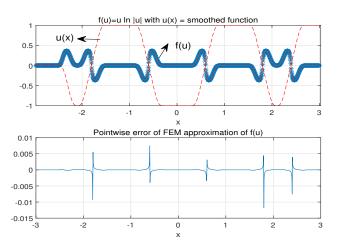
• Composition: g(x) = f(u(x)):

$$g'(x) = f'(u)u'(x) = (1 + \ln|u(x)|)u'(x), u \neq 0 \text{ or } u'(x) \neq 0.$$

• Composition: g(x) = f(u(x)):

$$g'(x) = f'(u)u'(x) = (1 + \ln|u(x)|)u'(x), \quad u \neq 0 \text{ or } u'(x) \neq 0.$$

• Maximum point-wise errors of FEM approximation (globally $\approx O(h)$) occur at the locations where u changes sign. Very localised!



Locally Holder Continuous

Lemma: Let $f(z) = z \ln |z|$ for $z \in \mathbb{R}$.

• If $0 \le |z_1| \le |z_2| \le \epsilon$ for $\epsilon > 0$, then for any $\alpha \in (0,1)$,

$$|f(z_1) - f(z_2)| \le (2\epsilon)^{1-\alpha} (|\ln \epsilon| + 1) |z_1 - z_2|^{\alpha},$$

i.e., α -Holder continuous on any finite interval containing 0.

8

Outline

- Examples and Motivations
- Existing Results: Theory & Numerics
- 3 Direct Linearised CN Scheme
- Positive and Ground-State Solutions
- 5 Numerical Results

Log-PDE: H^1 -Regularity or More?

Consider, for example, the Log-Heat equation:

$$\begin{cases} u_t - \Delta u = u \ln |u| & \text{in } \Omega, \ t > 0, \\ u(x,t) = 0 & \text{at } \partial \Omega, \ t \geq 0; \quad u(x,0) = u_0(x) \text{ on } \bar{\Omega}, \end{cases}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with a smooth boundary.

Log-PDE: H^1 -Regularity or More?

Consider, for example, the Log-Heat equation:

$$\begin{cases} u_t - \Delta u = u \ln |u| & \text{in } \Omega, \ t > 0, \\ u(x,t) = 0 & \text{at } \partial \Omega, \ t \ge 0; \quad u(x,0) = u_0(x) \text{ on } \bar{\Omega}, \end{cases}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with a smooth boundary.

● Global H^1 -solution (cf. Chen-Luo-Liu'15): $u \in L^\infty(0,\infty; H^1_0(\Omega))$ and $u_t \in L^2(0,\infty; L^2(\Omega))$, if $u_0 \in H^1_0(\Omega), J[u_0] < (2\pi)^{d/2}e^d/4$, and $I[u_0] \ge 0$, where ("Energy" has no definite sign \odot)

$$I[u] \coloneqq \|\nabla u\|^2 - \int_{\Omega} |u|^2 \frac{\ln |u|^2}{dx}, \quad J[u] = \frac{1}{2} I[u] + \frac{1}{4} \|u\|^2.$$

Log-PDE: H^1 -Regularity or More?

Consider, for example, the Log-Heat equation:

$$\begin{cases} u_t - \Delta u = u \ln |u| & \text{in } \Omega, \ t > 0, \\ u(x,t) = 0 & \text{at } \partial \Omega, \ t \ge 0; \quad u(x,0) = u_0(x) \text{ on } \bar{\Omega}, \end{cases}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with a smooth boundary.

● Global H^1 -solution (cf. Chen-Luo-Liu'15): $u \in L^\infty(0,\infty; H^1_0(\Omega))$ and $u_t \in L^2(0,\infty; L^2(\Omega))$, if $u_0 \in H^1_0(\Omega), J[u_0] < (2\pi)^{d/2}e^d/4$, and $I[u_0] \ge 0$, where ("Energy" has no definite sign \odot)

$$I[u] := \|\nabla u\|^2 - \int_{\Omega} |u|^2 \ln |u|^2 dx, \quad J[u] = \frac{1}{2} I[u] + \frac{1}{4} \|u\|^2.$$

• Blowup (cf. Han'19): If $u_0 \in H^1_0(\Omega)$ and $I[u_0] < 0$, $||u(\cdot,t)|| \to \infty$ as $t \to \infty$.

• Super-exponential decay/growth (cf. Alfaro-Carles'17): There exists $u_0 \in H_0^1$ with some $\eta > 0$, such that the unique solution decays super-exponentially

$$||u(\cdot,t)||_{\infty} \le Ce^{-\eta e^t}.$$

Moreover, there exist $u_0 \in H_0^1$ and $\exists \xi > 0$, s.t.

$$||u(\cdot,t)||_{\infty} \ge Ce^{\xi e^t}.$$

• Remark: Some recent results on LogSE, e.g., H^1 -regularity (cf. Carles-Gallagher'18)³, but no much on numerical methods.

 $^{^3}$ R. Carles and I. Gallagher, Universal dynamics for the defocusing logarithmic Schrödinger equation, Duke Math. J., 2018.

Regularized Numerical Methods

• Bao-Carles-Su-Tang (SINUM'19): Regularized LogSE:

$$\begin{cases} \mathrm{i} u_t^\varepsilon(x,t) + \Delta u^\varepsilon(x,t) = \lambda u^\varepsilon(x,t) \ln(\varepsilon + |u^\varepsilon(x,t)|) & \text{in } \Omega, \ t>0, \\ u^\varepsilon(x,t) = 0 \ \text{ at } \partial\Omega, \ t\geq0; \quad u^\varepsilon(x,0) = u_0(x) \ \text{ on } \bar{\Omega}. \end{cases}$$

Regularized Numerical Methods

Bao-Carles-Su-Tang (SINUM'19): Regularized LogSE:

$$\begin{cases} \mathrm{i} u_t^\varepsilon(x,t) + \Delta u^\varepsilon(x,t) = \lambda u^\varepsilon(x,t) \ln(\varepsilon + |u^\varepsilon(x,t)|) & \text{in } \Omega, \ t>0, \\ u^\varepsilon(x,t) = 0 & \text{at } \partial\Omega, \ t\geq0; \quad u^\varepsilon(x,0) = u_0(x) & \text{on } \bar{\Omega}. \end{cases}$$

• Regularization error: If $u_0 \in H^2(\Omega)$, then

$$\|u^\varepsilon-u\|_{L^\infty(0,T;L^2(\Omega))}\leq C_1\varepsilon,\quad \|u^\varepsilon-u\|_{L^\infty(0,T;H^1(\Omega))}\leq C_2\sqrt{\varepsilon},$$

where $C_1, C_2 > 0$ are independent of ε .

Crank-Nicolson-Leap-Frog in time with FD in space:

Theorem 3.1 (main result). Assume that the solution u^{ε} is smooth enough over $\Omega_T := \Omega \times [0,T]$, i.e.,

$$(A) \qquad \qquad u^{\varepsilon} \in C\left([0,T];H^{5}(\Omega)\right) \cap C^{2}\left([0,T];H^{4}(\Omega)\right) \cap C^{3}\left([0,T];H^{2}(\Omega)\right),$$

and there exist $\varepsilon_0 > 0$ and $C_0 > 0$ independent of ε such that

$$\|u^{\varepsilon}\|_{L^{\infty}(0,T;H^{5}(\Omega))} + \|\partial_{t}^{2}u^{\varepsilon}\|_{L^{\infty}(0,T;H^{4}(\Omega))} + \|\partial_{t}^{3}u^{\varepsilon}\|_{L^{\infty}(0,T;H^{2}(\Omega))} \leq C_{0},$$

uniformly in $0 \le \varepsilon \le \varepsilon_0$. Then there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small with $h_0^2 \sim \varepsilon e^{-CT |\ln(\varepsilon)|^2}$ and $\tau_0^2 \sim \varepsilon e^{-CT |\ln(\varepsilon)|^2}$ such that, when $0 < h \le h_0$ and $0 < \tau \le \tau_0$ satisfying the stability condition (3.7), we have the following error estimates

(3.9)
$$\|e^{\varepsilon,k}\| \le C_3(\varepsilon,T)(h^2 + \tau^2), \qquad 0 \le k \le \frac{T}{\tau},$$

$$\|e^{\varepsilon,k}\|_{H^1} \le C_4(\varepsilon,T)(h^2 + \tau^2), \quad \|u^{\varepsilon,k}\|_{\infty} \le \Lambda + 1,$$

where $\Lambda = \|u^{\varepsilon}\|_{L^{\infty}(\Omega_T)}$, $C_3(\varepsilon,T) \sim e^{CT|\ln(\varepsilon)|^2}$, $C_4(\varepsilon,T) \sim \frac{1}{\varepsilon}e^{CT|\ln(\varepsilon)|^2}$, and C depends on C_0 .

$$||u^n - u_h^{\varepsilon,n}|| \le e^{C_{\varepsilon}T(\ln \varepsilon)^2}(\varepsilon + \tau^2 + h^2).$$

Crank-Nicolson-Leap-Frog in time with FD in space:

Theorem 3.1 (main result). Assume that the solution u^{ε} is smooth enough over $\Omega_T := \Omega \times [0, T]$, i.e.,

(A)
$$u^{\varepsilon} \in C\left([0,T]; H^{5}(\Omega)\right) \cap C^{2}\left([0,T]; H^{4}(\Omega)\right) \cap C^{3}\left([0,T]; H^{2}(\Omega)\right),$$

and there exist $\varepsilon_0 > 0$ and $C_0 > 0$ independent of ε such that

$$\|u^{\varepsilon}\|_{L^{\infty}(0,T;H^{5}(\Omega))}+\|\partial_{t}^{2}u^{\varepsilon}\|_{L^{\infty}(0,T;H^{4}(\Omega))}+\|\partial_{t}^{3}u^{\varepsilon}\|_{L^{\infty}(0,T;H^{2}(\Omega))}\leq C_{0},$$

uniformly in $0 \le \varepsilon \le \varepsilon_0$. Then there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small with $h_0^2 \sim \varepsilon e^{-CT |\ln(\varepsilon)|^2}$ and $\tau_0^2 \sim \varepsilon e^{-CT |\ln(\varepsilon)|^2}$ such that, when $0 < h \le h_0$ and $0 < \tau \le \tau_0$ satisfying the stability condition (3.7), we have the following error estimates

(3.9)
$$\|e^{\varepsilon,k}\| \le C_3(\varepsilon,T)(h^2 + \tau^2), \qquad 0 \le k \le \frac{T}{\tau},$$

$$\|e^{\varepsilon,k}\|_{H^1} \le C_4(\varepsilon,T)(h^2 + \tau^2), \quad \|u^{\varepsilon,k}\|_{\infty} \le \Lambda + 1,$$

where $\Lambda = \|u^{\varepsilon}\|_{L^{\infty}(\Omega_T)}$, $C_3(\varepsilon,T) \sim e^{CT|\ln(\varepsilon)|^2}$, $C_4(\varepsilon,T) \sim \frac{1}{\varepsilon}e^{CT|\ln(\varepsilon)|^2}$, and C depends on C_0 .

$$||u^n - u_h^{\varepsilon,n}|| \le e^{C_{\varepsilon}T(\ln \varepsilon)^2}(\varepsilon + \tau^2 + h^2).$$

• Bao-Carles-Su-Tang (Numer. Math.'19): Regularized Lie-Trotter time splitting method: L^2 -error bound: $O(\tau^{\frac{1}{2}} \ln \varepsilon^{-1})$.

Outline

- Examples and Motivations
- Existing Results: Theory & Numerics
- Oirect Linearised CN Scheme
- Positive and Ground-State Solutions
- **5 Numerical Results**

Our Approach & Error Analysis

• Time discretization: Find $U^{n+1} \in H_0^1(\Omega)$ for $0 \le n \le N_t - 1$, s.t.

$$\frac{U^{n+1}-U^n}{\tau}-\Delta\Big(\frac{U^{n+1}+U^n}{2}\Big)=\lambda U^n\ln|U^n|\quad \text{in } \Omega,$$

with $U^0 = u_0$. FD, FEM or spectral method can be used in space.

- Remarks
 - It is first-order discretized at $t = t_n$. If $u_0 \equiv 0$, then $U^{n+1} \equiv 0$.

Our Approach & Error Analysis

• Time discretization: Find $U^{n+1} \in H_0^1(\Omega)$ for $0 \le n \le N_t - 1$, s.t.

$$\frac{U^{n+1}-U^n}{\tau}-\Delta\Big(\frac{U^{n+1}+U^n}{2}\Big)=\lambda U^n\ln|U^n|\quad \text{in } \Omega,$$

with $U^0 = u_0$. FD, FEM or spectral method can be used in space.

Remarks

- It is first-order discretized at $t = t_n$. If $u_0 \equiv 0$, then $U^{n+1} \equiv 0$.
- The non-differentiability of the log-term is not in favour of extrapolation or Newton iteration (for an implicit scheme).

Our Approach & Error Analysis

• Time discretization: Find $U^{n+1} \in H_0^1(\Omega)$ for $0 \le n \le N_t - 1$, s.t.

$$\frac{U^{n+1}-U^n}{\tau}-\Delta\Big(\frac{U^{n+1}+U^n}{2}\Big)=\lambda U^n\ln|U^n|\quad \text{in } \Omega,$$

with $U^0 = u_0$. FD, FEM or spectral method can be used in space.

Remarks

- It is first-order discretized at $t = t_n$. If $u_0 \equiv 0$, then $U^{n+1} \equiv 0$.
- The non-differentiability of the log-term is not in favour of extrapolation or Newton iteration (for an implicit scheme).
- Higher-order schemes can be used for e.g., positive, regular solutions.

Essential Tools for Error Analysis

• Theorem (Locally Holder Continuity, W.-Yan'22)

Let
$$f(z) = z \ln |z|$$
. If $u, v \in L^{\infty}(\Omega)$, then for any $\epsilon > 0$ and any $\alpha \in (0, 1)$,

$$||f(u) - f(v)|| \le (2\epsilon)^{1-\alpha} (|\ln \epsilon| + 1) ||u - v||^{\alpha}$$
$$+ (\max_{\epsilon \le z \le \Lambda_{\infty}} \{|\ln z| + 1\}) ||u - v||$$

where $\|\cdot\|$ is the L^2 -norm and

$$\Lambda_{\infty} \coloneqq \max\{\|u\|_{\infty}, \|v\|_{\infty}\}.$$

Lemma (Nonlinear Gronwall's inequality, W.-Yan'22)

Let c_1, c_2, c_3 be positive constants, and let $\{y(n)\}$ satisfy

$$y(n) \le c_1 + c_2 \sum_{m=0}^{n-1} y^{\alpha}(m) + c_3 \sum_{m=0}^{n-1} y(m), \quad n \ge 1, \ \alpha \in (0,1].$$

Then for any $\alpha \in (0,1]$,

$$y(n) \le c_1 \left(1 + \left(c_1^{\alpha - 1} c_2 + c_3 \right) \frac{\left(1 + \alpha c_1^{\alpha - 1} c_2 + c_3 \right)^n - 1}{\alpha c_1^{\alpha - 1} c_2 + c_3} \right), \quad n \ge 1.$$

• Lemma (Nonlinear Gronwall's inequality, W.-Yan'22)

Let c_1, c_2, c_3 be positive constants, and let $\{y(n)\}$ satisfy

$$y(n) \le c_1 + c_2 \sum_{m=0}^{n-1} y^{\alpha}(m) + c_3 \sum_{m=0}^{n-1} y(m), \quad n \ge 1, \ \alpha \in (0,1].$$

Then for any $\alpha \in (0,1]$,

$$y(n) \le c_1 \left(1 + \left(c_1^{\alpha - 1} c_2 + c_3 \right) \frac{\left(1 + \alpha c_1^{\alpha - 1} c_2 + c_3 \right)^n - 1}{\alpha c_1^{\alpha - 1} c_2 + c_3} \right), \quad n \ge 1.$$

Remarks

- (i) If $\alpha = 1$, it reduces to the linear Gronwall's inequality.
- (ii) A similar continuous integral version also holds.

• Lemma (Log-Sobolev inequality, Gross'76) If $u \in H_0^1(\Omega)$, then for any a > 0,

$$2\int_{\Omega} |u(x)|^2 \ln \left(\frac{|u(x)|}{\|u\|}\right) dx + d(1+\ln a) \|u\|^2 \le \frac{a^2}{\pi} \|\nabla u\|^2,$$

or equivalently,

$$\int_{\Omega} u^2 \ln u^2 dx + \left(d(1 + \ln a) - \ln \|u\|^2 \right) \|u\|^2 \le \frac{a^2}{\pi} \|\nabla u\|^2.$$

Main Result: FEM in Space

Theorem [Log-Heat] (W.-Yan'22): Under the condition of global existence as in Chen et al.'15, we further assume that the solution of the Log-Heat equation has the regularity:

$$u \in C^{2}([0,T];L^{2}(\Omega)) \cap C^{1}([0,T];H^{2}(\Omega)), \tag{1}$$
and $(\ln \tau)^{2} + (\ln |\ln h|)^{2} \le c$, then for $\alpha \in (1/2,1)$,
$$\|u^{n} - u_{h}^{n}\| \le C_{\tau}(\tau + h^{2\alpha}), \quad C_{\tau} \sim e^{cT(\ln \tau)^{2}}.$$

Main Result: FEM in Space

Theorem [Log-Heat] (W.-Yan'22): Under the condition of global existence as in Chen et al.'15, we further assume that the solution of the Log-Heat equation has the regularity:

$$u \in C^2([0,T]; L^2(\Omega)) \cap C^1([0,T]; H^2(\Omega)),$$
 (1)

and $(\ln \tau)^2 + (\ln |\ln h|)^2 \le c$, then for $\alpha \in (1/2, 1)$,

$$||u^n - u_h^n|| \le C_\tau (\tau + h^{2\alpha}), \quad C_\tau \sim e^{cT(\ln \tau)^2}.$$

Remarks:

- ullet Used the argument for parabolic problems by introducing an auxiliary semi-discretised elliptic problem of U^n as in B. Li-W. Sun'13.
- The extra log-factor appears inevitable, but seems insignificant.

Theorem (LogSE): Assume the regularity condition (1) holds, and

$$C_1 h^{2\alpha} \le \tau \le C_2 h^{d/2}, \quad (\ln \tau)^2 + (\ln |\ln h|)^2 \le C_3.$$
 (2)

Then we have that for $\alpha \in (1/2, 1)$,

$$||u^n - u_h^n|| \le C_\tau (\tau + h^{2\alpha}), \quad C_\tau \sim e^{cT(\ln \tau)^2}.$$

Theorem (LogSE): Assume the regularity condition (1) holds, and

$$C_1 h^{2\alpha} \le \tau \le C_2 h^{d/2}, \quad (\ln \tau)^2 + (\ln |\ln h|)^2 \le C_3.$$
 (2)

Then we have that for $\alpha \in (1/2, 1)$,

$$||u^n - u_h^n|| \le C_\tau (\tau + h^{2\alpha}), \quad C_\tau \sim e^{cT(\ln \tau)^2}.$$

Remark:

- The argument of Li-Sun'13 and J. Wang'14 cannot be applied due to the non-differentiability of the logarithmic nonlinear term.
- This led to the conditions in (2) largely from the use of inverse inequality.
- Compared with regularized approach, the conditions are on the original PDEs (at least positive solutions having such regularity).

Outline

- Examples and Motivations
- Existing Results: Theory & Numerics
- 3 Direct Linearised CN Scheme
- Positive and Ground-State Solutions
- Numerical Results

Motivations

The LogSE for N particles (Bialynicki et al' 1979):

$$\mathrm{i}\hbar \,\partial_t \psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N,t) = \left[-\,\hbar^2 \sum_{k=1}^N \frac{1}{2m_k} \Delta_k - b \ln\left(|\psi|^2 a^{3N}\right)\right] \psi(\boldsymbol{r}_1\ldots,\boldsymbol{r}_N,t),$$

• Dimensionless LogSE in d = 3N dimensions

$$i\partial_t \Psi(\boldsymbol{r},t) = \left[-\Delta - \ln |\Psi|^2 \right] \Psi(\boldsymbol{r},t), \quad \boldsymbol{r} \in \mathbb{R}^{3N},$$
 (3)

where Ψ = $a^{3N/2}\psi$ and

$$r = \hbar^{-1}\sqrt{2b}\left(r_1\sqrt{m_1}\ldots,r_N\sqrt{m_N}\right).$$

• Time-harmonic problem: if $\Psi({\bf r},t)=e^{\frac{\omega}{2\lambda}-i\omega t}u({\bf r})$ is a solution of (3), then

$$-\Delta u(\mathbf{r}) + \lambda u(\mathbf{r}) \ln |u(\mathbf{r})|^2 = 0, \quad \mathbf{r} \in \mathbb{R}^d.$$
 (4)

The problem of finding a positive ground state solution u > 0,

$$\Delta u + u \ln |u| = 0$$
 in \mathbb{R}^d , $u \to 0$, $r = |x| \to +\infty$

is of fundamental importance.

• It has a unique solution $u(r) = \exp(d/2 - r^2/4) > 0$ if $d \in [1, 9]$ (cf. Troy'16): Ground-state solution:

$$E(v) = \|\nabla v\|^2 - \int_{\mathbb{R}^d} |v|^2 \ln |v|^2 dx \ge E[u] = d(1 + \ln \pi/2).$$

• Related to the steady state problem of nonlinear Klein-Gordon and parabolic equations as $p \rightarrow 0^+$:

$$u_{tt} = \Delta u + u|u|^p - u, \quad u_t = \Delta u + u|u|^p - u$$

Remark: The existence of positive solutions for the above was studied e.g., by Berestycki-Lions'83, Coffman'96, etc..

- Our Goal: Find analytically or compute numerically positive solutions in more general setting, e.g., with a potential *V*.
- For example, we consider the steady-state problem:

$$-\Delta u + Vu = \lambda u \ln|u|, \quad u > 0 \tag{5}$$

We also consider time-dependent problems, e.g.,

$$u_t - \Delta u + Vu = \lambda u \ln |u|, \quad u > 0$$
 (6)

 Ideally to design positivity-preserving schemes, but non-trivial for some schemes.

Our Approach: Exponential Substitution

- Introduce the exponential substitution: $u = e^v > 0.4$
- It favours the log-term:

$$u \ln |u| = uv$$
, $u_t = uv_t$, $\Delta u = u(\Delta v + |\nabla v|^2)$

The steady-state equation (5) reads

$$\Delta v + |\nabla v|^2 + \lambda v = V \tag{7}$$

• The time-dependent problem (6) becomes

$$v_t - (\Delta v + |\nabla v|^2) - \lambda v = -V \tag{8}$$

⁴Huang-Shen (SISC'21) introduced the exponential substitution for constructing positivity preserving schemes for Poisson-Nernst-Planck (PNP) equations.

Selected Analytic Solutions

• If V = V(r), we seek the axis-symmetric solution of

$$v'' + \frac{d-1}{r}v' + (v')^2 + \lambda v = V(r), \quad r > 0$$

• For example, if $V = \kappa r^{-1}$ (Coulomb's potential), then

$$u(r) = \exp\left(-\frac{\lambda}{4}r^2 + \frac{\kappa}{\varepsilon^2(d-1)}r - \frac{\kappa^2}{\lambda(d-1)^2} + \frac{d}{2}\right), \quad d \ge 2, \lambda > 0.$$

• We can also find Gaussian solutions for polynomial $V = \kappa |x|^m$ when m = 0, 1, 2, or more general

$$V(r) = \kappa_1 r^2 + \kappa_2 r + \kappa_3 + \kappa_4 r^{-1}, \quad V(r) = \lambda a_2 \log r + a_2 (a_2 + d - 2) r^{-2}.$$

• We can show some solutions are ground-state, but some are excited state solutions for respective V(r).

• Time-dependent problem (8) with $V = \kappa |x|^m$ has the analytic positive solution $u(r,t) = e^{v(r,t)}$ with

$$v(r,t) = A(t)e^{\lambda t} + B(t)P(r), \quad P(r) = r^2 + \alpha,$$
 (9)

where A, B can be solved out from some solvable ODEs.

- The same techniques can be applied to study the LogSE with $V = \kappa |x|^m$ that can enrich the studies by Carles-Ferriere'21.
- Computing positive solutions for initial-valued BVPs in more general setting (Ongoing)!

Outline

- Examples and Motivations
- Existing Results: Theory & Numerics
- 3 Direct Linearised CN Scheme
- Positive and Ground-State Solutions
- Numerical Results

Numerical Results: Accuracy Test

• Scheme: Find $u_h^{n+1} \in V_h^0$ for $0 \le n \le N_t - 1$, s.t.

$$\left(\frac{u_h^{n+1}-u_h^n}{\tau},v_h\right)+\left(\nabla\left(\frac{u_h^{n+1}+u_h^n}{2}\right),\nabla v_h\right)=\left(\lambda u_h^n\ln|u_h^n|,v_h\right),\quad\forall v_h\in V_h^0,$$
 with $u_h^0=I_hu_0$.

• Test the positive (smooth) exact solution given in (9), and expect to get the optimal order: $O(\tau + h^2)!$

Table 1: Piecewise Linear FEM $(h = 2^{-M}, \tau = h^2, T = 1)$

\overline{M}	$\ e\ _2$	Order	$\ e\ _{\infty}$	Order
4	4.43e -3	-	5.91e -3	-
8	1.02e -3	2.12	1.41e -3	2.07
16	2.47e- 4	2.05	3.47e-4	2.02
32	6.08e-5	2.02	8.65e- 5	2.00
64	1.51e -5	2.01	2.16e- 5	2.00
128	3.77e- 6	2.00	5.40e- 6	2.00

Table 2: Piecewise Quadratic FEM ($h = 2^{-M}$, $\tau = h^3$, T = 1)

M	$\ e\ _2$	Order	$\ e\ _{\infty}$	Order
2	8.05e -3	-	9.93e -3	-
4	8.65e-4	3.22	1.21e -3	3.03
8	1.00e -4	3.11	1.52e- 4	2.99
16	1.21e -5	3.06	1.91e -5	3.00
32	1.48e -6	3.03	2.37e-6	3.00
64	1.83e-7	3.01	2.96e-7	3.00

Spectral Methods in Space

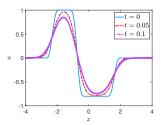
Table 3: Convergence order in space ($\tau = 1 \times 10^{-5}, T = 1$)

N	$\ e\ _2$	Order	$\ e\ _{\infty}$	Order
20	8.16e- 3	-	8.16 e-3	-
24	3.91e-3	4.04	3.91e -3	4.21
28	1.66e- 3	5.57	1.66e- 3	5.80
32	6.21e -4	7.34	6.21e -4	7.58
36	2.07e-4	9.32	2.07e-4	9.56
40	6.19e- 5	11.48	6.19e -5	11.71
44	1.66e- 5	13.82	1.66e- 5	13.98
48	4.00e-6	16.33	4.00e-6	16.09

Table 4: Convergence order in time ($N = 2^{10}, T = 1$)

τ = 1.25e-3	$\ e\ _2$	Order	$\ e\ _{\infty}$	Order
au	1.02e-3	-	1.02e-3	-
$\tau/2^1$	5.12e-4	1.00	5.04e-3	1.00
$\tau/2^2$	2.56e-4	1.00	2.52e- 4	1.00
$\tau/2^3$	1.28e- 4	1.00	1.26e- 4	1.00
$\tau/2^4$	6.41e-5	1.00	6.31e -4	1.00
$\tau/2^5$	3.21e- 5	1.00	3.16e- 5	1.00

Non-positive Solutions: H^{1+} -Regularity



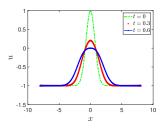


Table 5: Convergence in space (it is first-order in time)

\overline{N}	$ e _2$	Order	$\ e\ _{\infty}$	Order
2^{6}	2.96e-2	-	2.16e-2	-
2^7	1.45e-2	1.03	1.09e-2	0.99
2^{8}	6.93e-3	1.07	5.19e-3	1.06
2^{9}	3.25e-3	1.09	2.43e-3	1.09
2^{10}	1.39e-3	1.22	1.04e-3	1.22

Table 6: Convergence in space (it is first-order in time)

N	$ e _2$	Order	$ e _{\infty}$	Order
$^{2^{6}}$	8.01e-2	-	8.01e-2	-
2^7	4.35e-2	0.94	4.35e-2	0.88
2^{8}	1.64e-2	1.55	1.64e-2	1.41
2^{9}	8.11e-3	1.10	8.11e-3	1.01
2^{10}	3.48e-3	1.22	3.48e-3	1.22

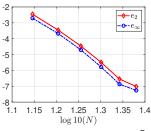
Numerical Results on LogSE

We test the numerical scheme on the LogSE:

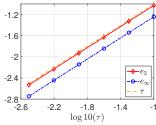
$$iu_t + \Delta u = \lambda u \ln |u|, \quad t > 0; \quad u(x,0) = u_0(x),$$

with the exact Gaussian solution:

$$u(x,t) = b_0 e^{\frac{\lambda}{2}(x-2vt)^2 + i(vx-(\phi_0+v^2)t)}, \quad t \ge 0.$$



(a) Spatial Conv.: $\tau = 10^{-7}$



(b) Temporal Conv.: N = 256

Take the initial data:

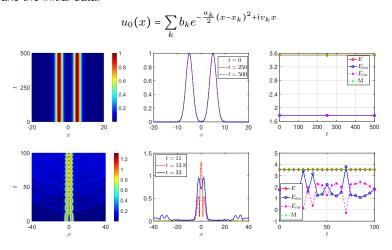


Figure 1: $\sqrt{|u(x,t)|}$, |u(x,t)| and energies & mass at different time: (i) $x_1 = -x_2 = -5$, $v_k = 0$, $b_k = a_k = 1$; (ii) $x_1 = -x_2 = -3$, $v_k = 0$, $b_k = a_k = 1$.

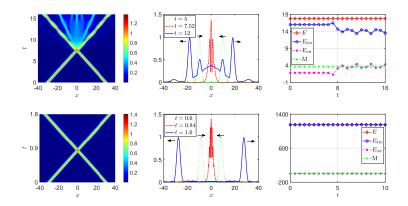


Figure 2: $\sqrt{|u(x,t)|}$, |u(x,t)| and energies & mass at different time:

(iii)
$$v_1 = -v_2 = 2, x_1 = -x_2 = -30, b_k = a_k = 1(k = 1, 2);$$

(iv)
$$v_1 = 18, v_2 = -18, x_1 = -30, x_2 = 30, b_2 = b_1 = 1, a_1 = a_2 = 1.$$

Mass Preserving Scheme (ongoing)

- IMEX Relaxed Runge-Kutta Scheme:
 - Step 1: Find \tilde{u}^{n+1} through BDF1:

$$i\frac{\tilde{u}^{n+1} - u^n}{\tau} + \Delta \tilde{u}^{n+1} = \lambda f(u^n). \tag{10}$$

• Step 2: Find u^{n+1} through correction:

$$u^{n+1} = u^n + i\tau \gamma_n (\Delta \tilde{u}^{n+1} - \lambda f(\tilde{u}^{n+1})). \tag{11}$$

Relaxation parameter:

$$\gamma_{n} = \begin{cases} 1, & \|\Delta \tilde{u}^{n+1} - \lambda f(\tilde{u}^{n+1})\| = 0, \\ \frac{2 \operatorname{Im}\{(\Delta \tilde{u}^{n+1} - \lambda f(\tilde{u}^{n+1}), u^{n})\}}{\tau \|\Delta \tilde{u}^{n+1} - \lambda f(\tilde{u}^{n+1})\|^{2}}, & \|\Delta \tilde{u}^{n+1} - \lambda f(\tilde{u}^{n+1})\| \neq 0. \end{cases}$$
(12)

We have

$$||u^{n+1}||^2 = ||u^n||^2. (13)$$

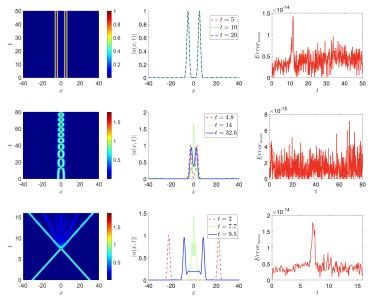


Figure 3.1: Plots of |u(x,t)| (first column); |u(x,t)| at different time (second column) and evolution of mass error (third column).

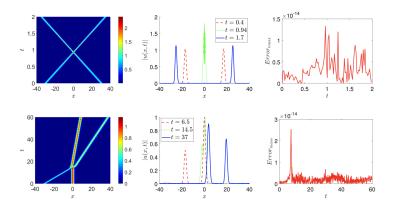


Figure 3.1: Plots of |u(x,t)| (first column); |u(x,t)| at different time (second column) and evolution of mass error (third column).

Summary

- The non-differentiability of logarithmic nonlinear term needs special care in discretisation.
- New tools were introduced for the analysis, though the results might not be the best at this moment.
- Exponential substitution is a feasible and simpler way to study and compute the positive solutions.
- Many issues are under-explored, e.g., fractional LogSE in space, time-fractional LogSE(?), Stay tuned!

