The initial-boundary value problem for the Lifshitz–Slyozov system with inflow boundary conditions

J. Calvo, E. Hingant, R. Yvinec

Universidad de Granada

SIAM Materials 2021,
17-28 May 2021, Bilbao and elsewhere

The Lifshitz–Slyozov model

$$\begin{cases} \dfrac{\partial f(t,x)}{\partial t} + \dfrac{\partial}{\partial x}[(a(x)u(t) - b(x))f(t,x)] = 0\,, \quad t > 0\,,\ x \in (0,\infty)\,, \\ u(t) + \displaystyle\int_0^{\infty} x\, f(t,x)\, dx = \rho\,,\ t > 0, \quad \text{plus an initial condition } f^{in}(x) \end{cases}$$

- The ***aggregate* distribution** $0 \le f(t,x)$ as a function of size x and time t.
- The ***monomer* concentration** $0 \le u(t)$.
- The **total mass** of the system, $\rho > 0$.

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$$\text{aggregate number} = \int_0^\infty f(t,x)\, dx$$

$$\text{total aggregate size} = \int_0^\infty x\, f(t,x)\, dx$$

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- The ***aggregate* distribution** $0 \leq f(t,x)$ as a function of size x and time t.
- The ***monomer* concentration** $0 \leq u(t)$.
- The **total mass** of the system, $\rho > 0$.
- The **kinetic rates** $a(x)$ and $b(x)$, describing how fast do reactions take place:
  - *attachment* (a monomer attaches to a given aggregate)
  - *detachment* (a monomer detaches from a given aggregate)

Lifshitz–Slyozov's model: the classical rates

$$a(x) = x^{1/3}, \quad b(x) = 1$$

Relative rate

$$\Phi(x) = \frac{b(x)}{a(x)} \quad \text{and} \quad \Phi_0 = \lim_{x \to 0} \frac{b(x)}{a(x)}$$

Transport field:

$$v(t,x) = a(x)u(t) - b(x) = a(x)(u(t) - \Phi(x))$$

Ostwald ripening: large aggregates ($x > \Phi^{-1}(u(t))$) grow larger at the expense of smaller ones ($x < \Phi^{-1}(u(t))$).

Lifshitz–Slyozov's model: the classical rates

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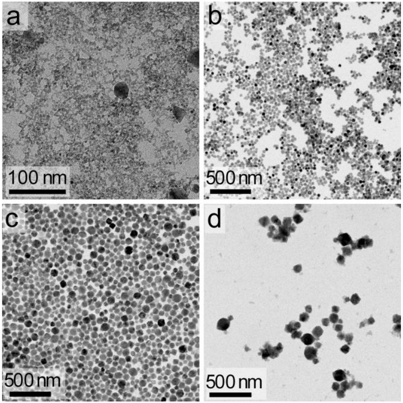


($LiNbO_3$ nanoparticles. Image: R. F. Ali, B. D. Gates, Chemistry of Materials 30 (2018))

Lifshitz–Slyozov's model: some existence results

- $a(x)$ and $b(x)$ are globally Lipschitz.
- $a(x) \geq 0$ and $b(x) > 0$ for every $x \geq 0$.
- (**outflow assumption**) $a(0)\rho - b(0) \leq 0$.

Theorem [Collet-Goudon]

Under the given assumptions, let $f^{in} \geq 0$ be such that

$$\int_0^\infty f^{in}(x)\, dx < \infty, \quad \int_0^\infty x\, f^{in}(x)\, dx \leq \rho.$$

Then the Lifshitz–Slyozov system has a unique global solution with f^{in} as initial datum. [incidentally when $a(0) = b(0) = 0$ we do not need f^{in} to be integrable]

Superlinear behavior for the rates can lead to solutions that blow up in finite time.

Lifshitz–Slyozov's model: some existence results

- $a(x) = a_M + a_L$ and $b(x) = b_M + b_L$.
- a_M, b_M nondecreasing and Lipschitz out of the origin.
- a_L, b_L globally Lipschitz and vanishing at the origin.
- (**outflow assumption**) $\rho a_M(x) - b_M(x) \leq -x\, b'_M(x)$ around the origin.

Theorem [Laurençot]

Under the given assumptions, let $f^{in} \geq 0$ be such that

$$\int_0^\infty x\, f^{in}(x)\, dx \leq \rho.$$

Then the Lifshitz–Slyozov system has a global weak solution with f^{in} as initial datum. With f^{in} integrable and a slightly stronger outflow assumption this solution is unique.

Lifshitz–Slyozov's model: some existence results

Measure solutions: results by Niethammer and Pego (also for the Lifshitz–Slyozov–Wagner model)

Global existence and uniqueness of distributional solutions that are probability measures with finite first moment for each t.

(B. Niethammer, R. L. Pego, Siam. J. Math. Anal. 31 (2000))

(B. Niethammer, R. L. Pego, Indiana Univ. Math. J. 54 (2005))

Their assumptions entail that $\Phi_0 = +\infty$ (outflow setting, Ostwald-ripening-like scenario).

Are we going to remain always in the outflow scenario?

Lifshitz–Slyozov's model: local-in-time solutions

- $\rho > \Phi_0 > u^{in}$
- Φ concave and non-constant
- $a(x)$ bounded and separated from zero

$\mathrm{supp}_x\, f(t)$ is contained in $[0, z(t))$ with $z(t) := C_1(1+t)$.

$$\Phi(x) \geq \Phi_0 + \frac{\Phi(z) - \Phi_0}{z} x \,, \ \forall\, 0 < x < z$$

$$\frac{du(t)}{dt} = \int_0^{z(t)} a(x)(\Phi(x) - u(t)) f(t,x)\, dx \geq 0$$

and *a fortiori*

$$\frac{du(t)}{dt} \geq \frac{C_2}{C_1(1+t)} \implies$$

Finite time crossing $u(t) \geq \Phi_0$!!!

Lifshitz–Slyozov's model: the inflow situation

$$\begin{cases} \dfrac{\partial f(t,x)}{\partial t} + \dfrac{\partial}{\partial x}[(a(x)u(t) - b(x))f(t,x)] = 0\,, \quad t > 0\,,\ x \in (0,\infty)\,, \\ u(t) + \displaystyle\int_0^\infty x\, f(t,x)\, dx = \rho\,,\ t > 0, \quad \text{plus an initial condition } f^{in}(x) \\ \lim_{x\to 0^+}(a(x)u(t) - b(x))f(t,x) = \mathfrak{n}(u(t))\,, \quad \text{whenever } u(t) > \Phi_0 \end{cases}$$

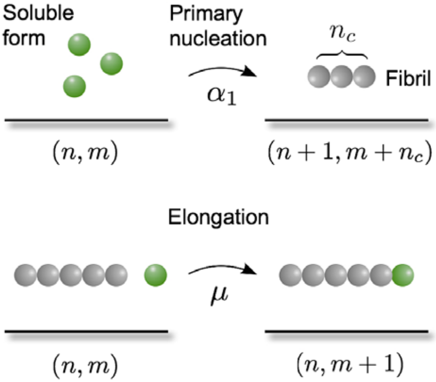
The boundary condition represents nucleation phenomena:

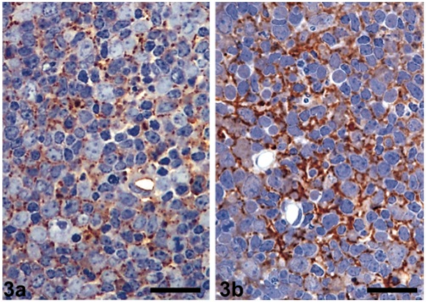
$$\frac{d}{dt}\int_0^\infty f(t,x)\,dx = \mathfrak{n}(u(t)) \quad \text{whenever } u(t) > \Phi_0.$$

Potentially wide range of applications:
encompass non-Lipschitz rates at the origin.

Lifshitz–Slyozov's model: the inflow situation

Application: protein polymerization and neurodegenerative diseases [e.g. works by M. Doumic and collaborators]

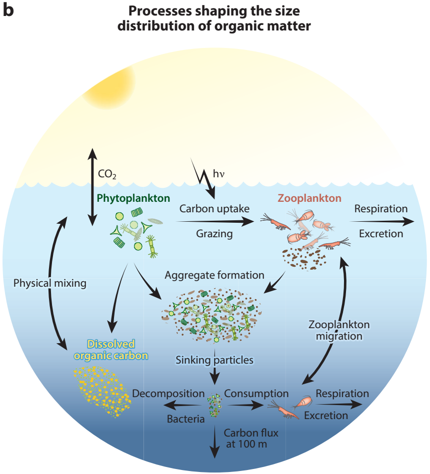




(Images: Michaels et al PRL 2016 - Gillian McGovern, Martin Jeffrey, Plos One)

Lifshitz–Slyozov's model: the inflow situation

Application: sea-surface microlayer



Benner, Amon, Annu. Rev. Mar. Sci. 2015

Figure 5: Redistribution of surface-associated OM and slick patterns by passage of a ship. Surface wake pattern 100 min after passage of a ship, showing contrast between undisturbed and disturbed surface film patterns. Remastered from Peltzer et al. (1992). DOI: https://doi.org/10.1525/elementa.283.f5

Lifshitz–Slyozov's model: the inflow situation

We consider kinetic rates $\{a, b, \mathfrak{n}\}$ that satisfy:

- $0 \leq a,\ b \in \mathcal{C}^0([0,\infty)) \cap \mathcal{C}^1(0,\infty)$,
- a' and b' are bounded on $(1,\infty)$,
- $a(x) > 0$ for all $x > 0$ and $\frac{1}{a} \in L^1(0,1)$,
- $\Phi' \in L^1(0,1)$,
- $0 \leq \mathfrak{n}$ is locally Lipschitz on $[\Phi_0,\infty)$.

We restrict the choice of initial data to

- $f^{\text{in}} \in L^1((0,\infty),(1+x)\,dx)$,
- $u^{\text{in}} := \rho - \int_0^\infty x\, f^{\text{in}} > \Phi_0$,

so that the balance of mass makes sense at time $t = 0$ and the flow has incoming character.

Lifshitz–Slyozov's model: the inflow situation

Theorem: existence of solutions

Let $\{a, b, \mathfrak{n}\}$, $\rho > \Phi_0$ and f^{in} satisfy our hypotheses. Then, there exists some $T > 0$ and a weak solution
$0 \leq f \in \mathcal{C}([0, T); w - L^1((0, \infty), (1 + x)\, dx))$
to the Lifshitz–Slyozov initial-boundary value problem.

This solution is such that:

- For each $T^* < T$, f belongs to $L^\infty((0, T^*), L^1((0, \infty), dx))$.
- It can be represented in terms of characteristics.

Moreover, if T is taken to be maximal then either $T = \infty$ or $T < \infty$ and $u(t) \to \Phi_0$ as $t \to T$.

(J. Calvo, E. Hingant, R. Yvinec, Nonlinearity 34 (2021))

Write $v(t,x) := a(x)u(t) - b(x)$ for the transport field

Linear problem

Given $u(t) > \Phi_0$ for $t \in [0,T)$ and f^{in}, solve for $t \in (0,T)$

$$\begin{cases} \dfrac{\partial f(t,x)}{\partial t} + \dfrac{\partial}{\partial x}[v(t,x)\, f(t,x)] = 0\,, \quad t > 0\,,\ x \in (0,\infty)\,, \\ \lim_{x\to 0^+}(a(x)u(t) - b(x))f(t,x) = \mathfrak{n}(u(t))\,. \end{cases}$$

Characteristics: for $(t,x)\in[0,T)\times(0,\infty)$, maximal solutions of

$$\begin{cases} \dfrac{dX(s;t,x)}{ds} = v(s, X(s;t,x))\,, \\ X(t;t,x) = x, \end{cases}$$

defined on the time interval $\Sigma_{t,x}$.

Lifshitz–Slyozov's model: the linearized problem

Characteristics: for $(t,x)\in[0,T)\times(0,\infty)$, maximal solutions of

$$\begin{cases} \dfrac{dX(s;t,x)}{ds} = v(s, X(s;t,x))\,, \\ X(t;t,x) = x, \end{cases}$$

defined on the time interval $\Sigma_{t,x}$.

The associated Jacobian is

$$J(s;t,x) = \exp\left(-\int_s^t (\partial_x v)(\tau, X(\tau;t,x))\,d\tau\right)\,.$$

Lifshitz–Slyozov's model: the linearized problem

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defined on the time interval $\Sigma_{t,x}$.

Tracking trajectories stemming from $x=0$:

- *enter-time* associated to the characteristic curve passing through (t,x)

  $$\sigma_t(x) := \inf \Sigma_{t,x}$$

  (time at which $s \mapsto (s, X(s;t,x))$ enters $(0,\infty)$).
- *separating point:* $x_c(t) := \inf\{x > 0 / \sigma_t(x) = 0\}$

Characteristics: defined on the time interval $\Sigma_{t,x}$.

$$\begin{cases} \dfrac{dX(s;t,x)}{ds} = v(s, X(s;t,x))\,, \\ X(t;t,x) = x, \end{cases}$$

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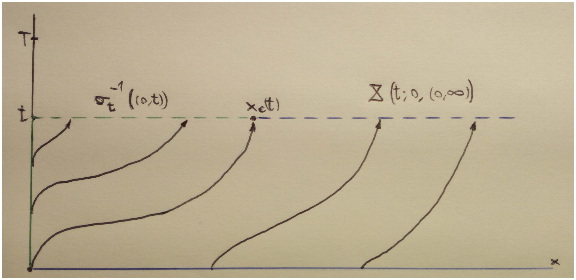


Lifshitz–Slyozov's model: the linearized problem

Eventual lack of uniqueness for $X(s;t,x)$ at $x=0$

- Spatial reparametrization: $A(x) := \int_0^x \frac{dy}{a(y)}$.
  This is an increasing diffeomorphism from $(0,\infty)$ into itself that extends to the origin.
- Reparametrized transport field: $V(t,x) := u(t) - \Phi \circ A^{-1}(x)$
- Associated trajectories for $(t,y) \in [0,T) \times (0,\infty)$:

$$\begin{cases} \dfrac{dB(s;t,y)}{ds} = V(s,B(s;t,y))\,, \\ B(t;t,y) = y, \end{cases}$$

$$B(s;t,A(x)) = A(X(s;t,x))$$

Lifshitz–Slyozov's model: the linearized problem

Proposition

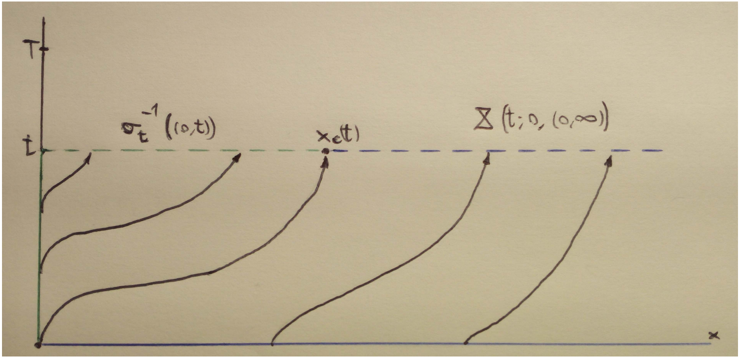
For each $t \in (0, T)$, the following holds:

- The map $x \mapsto X(t; 0, x)$ is an increasing $\mathcal{C}^1$-diffeomorphism from $(0, \infty)$ to $(x_c(t), \infty)$.
- The map $s \mapsto \sigma_t^{-1}(s)$ is a decreasing $\mathcal{C}^1$-diffeomorphism from $(0, t)$ to $(0, x_c(t))$.

(J.Calvo, E. Hingant, R. Yvinec, Nonlinearity 34 (2021))

$$f(t,x) = f^{\rm in}(X(0;t,x))J(0;t,x)\mathbf{1}_{(x_c(t),\infty)}(x)$$
$$+\mathfrak{n}(u(\sigma_t(x)))|\sigma_t'(x)|\mathbf{1}_{(0,x_c(t))}(x)\,.$$

Lifshitz–Slyozov's model: the linearized problem



$$f(t,x) = f^{\mathrm{in}}(X(0;t,x))J(0;t,x)\mathbf{1}_{(x_c(t),\infty)}(x) + \mathfrak{n}(u(\sigma_t(x)))|\sigma_t'(x)|\mathbf{1}_{(0,x_c(t))}(x)\,. \quad (1)$$

Lifshitz–Slyozov's model: local existence

Using the strategy of [*J.-F. Collet, T. Goudon, Nonlinearity 13 (2000)*] we prove existence by a fixed point argument on $u(t)$:

- Let $\delta > 0$ such that $2\delta < u^{in} - \Phi_0$.
- Define a map G on $\{u \in C([0,T))/\Phi_0 + \delta \leq u(t) \leq \rho\}$ by

$$u(t) \mapsto f(t,x) \mapsto \tilde{u}(t) = G(u)(t) = \max\left\{\Phi_0 + \delta,\ \rho - \int_0^\infty x\, f(t,x)\, dx\right\}$$

  where $f(t,x)$ solves the linearized problem with the given $u(t)$ and f^{in}.
- The regularity of characteristic trajectories entails the continuity of the fixed-point map G via (1).
- $\tilde{u}'(t)$ is uniformly bounded (via Dunford–Pettis). Then Schauder's fixed point theorem can be applied.

Lifshitz–Slyozov's model: uniqueness

Uniqueness

Let our running assumptions on the rates and initial data be satisfied. Assume that there exists $x^* > 0$ such that Φ is monotone on $[0, x^*)$. Then, for any given $T > 0$, there exists at most one weak solution to the inflow Lifshitz–Slyozov system on $(0, T)$ with the given initial data.

(J. Calvo, E. Hingant, R. Yvinec, Nonlinearity 34 (2021))

Proof by an adaptation of the technique introduced in [*P. Laurençot, Indiana Univ. Math. J. 50 (2001)*]:
we derive an evolution equation for quantities of the form

$$F^+(t,x) = \int_x^\infty f(t,y)\, dy \,.$$

Gronwall estimates $\implies$ uniqueness for these quantities.

Lifshitz–Slyozov's model: particular cases

Proposition (global existence)

Assume $\Phi(x) \geq \Phi_0$ for all $x > 0$. Then, the solution to the Lifshitz–Slyozov equation constructed in our existence theorem is global, that is $T = \infty$.

Proposition (finite-time existence)

Assume that f^{in} is compactly supported, that Φ is convex and strictly decreasing and that there exists numbers $\underline{a}$, $\overline{a}$ such that $0 < \underline{a} < a(x) < \overline{a} < \infty$ for all $x > 0$. Then, the solution to the Lifshitz–Slyozov equation constructed in our existence theorem is not global, that is, u reaches Φ_0 in finite time.

(J. Calvo, E. Hingant, R. Yvinec, Nonlinearity 34 (2021))

Recap

- The Lifshitz–Slyozov model with nucleation boundary conditions can be used to describe polymerization phenomena in different contexts.
- We provide a local existence result + representation formula under broad hypotheses.
- A continuation criterion is given, together with examples of both local and global solutions.

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FEDER
Fondo Europeo de Desarrollo Regional
UNIÓN EUROPEA
"Una manera de hacer Europa"

Grant MTM2017-91054-EXP

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