Thermodynamically Consistent and Positivity Preserving Discretization of the Stochastic Thin Film Equation

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joint work(s) with: Konstantinos Dareiotis, Manuel Gnann, Rishabh Gvalani, Florian Kunick, Felix Otto, Max Sauerbrey: [G., Gnann; SPA, 2020], [Dareiotis, G., Gnann, Grün; ARMA, 2021],**[G., Gvalani, Kunick, Otto; Math. Comp. 2023] [G., Otto, Sauerbrey, 2026+]**.

The deterministic thin film equation

Consider (thin) film of fluid on a $1d$-substrate

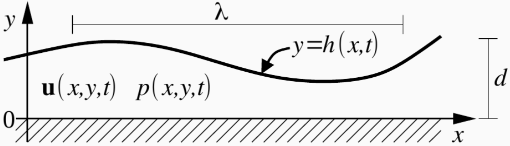


Figure 1: A thin liquid film on a flat one-dimensional substrate (coinciding with the x-axis). The film surface (i.e., the moving boundary) is parameterized by the film thickness $h(x,t)$. The flow is characterized by the flow velocity $\mathbf{u} = (u_x, u_y)$ and the pressure p. (source: Grün, Mecke, Rauscher, 2006)

Dynamics of the fluid: E.g. Navier-Stokes equations

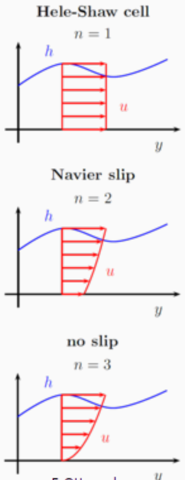
$$\partial_t u = \Delta u - (u \cdot \nabla)u - \nabla p, \quad \nabla \cdot u = 0.$$

Thin-film equation

- "Lubrication approximation": Derive PDE for h in the regime $\frac{d}{\lambda} << 1$. [Giacomelli, Otto; 2003]
- Thin film equation:

$$\partial_t h = -\partial_x \big(h^m \partial_{xxx} h \big) \quad \text{on } \mathbb{T},$$
$$\partial_t h = -\partial_x \big(M(h) \partial_{xxx} h \big) \quad \text{more generally.}$$

  with a free interface at $\partial\{h > 0\}$.
- Different fluid-solid boundary conditions $m \in [1, 3]$.



source: F. Otto webpage

Gradient flow stucture: The equation is written as

$$\partial_t h = -\partial_x\big(M(h)\partial_{xxx}h\big) = -\partial_x\Big(M(h)\partial_x \overbrace{\partial_{xx}h}^{-\delta\mathcal{E}/\delta h}\Big) = -\nabla_{\mathcal{M}}\mathcal{E}(h) = -G^{-1}(h)\frac{d\mathcal{E}}{dh}(h),$$

$G^{-1}(h) := -\partial_x\big(M(h)\partial_x\cdot\big)$.

Surface-tension / capillarity energy

$$\mathcal{E}(h) := \frac{1}{2}\int_0^1 (\partial_x h)^2\,\mathrm{d}x.$$

The discretization of the geometry does not rely on this particular choice. (Ginzburg Landau etc.)

The mobility $M : \mathbb{R}_+ \to \mathbb{R}_+$ determines the generalized Wasserstein-type geometry.

$$\mathcal{M} := \Big\{h : \mathbb{R} \to \mathbb{R} : h \text{ is 1-periodic, } h > 0,\ \int_0^1 h\,\mathrm{d}x = 1\Big\},$$

$$T_h\mathcal{M} := \Big\{\dot h : \mathbb{R} \to \mathbb{R} : \dot h \text{ is 1-periodic, } \int_0^1 \dot h\,\mathrm{d}x = 0\Big\}.$$

Informal geometry and energy

For $\dot h \in T_h\mathcal{M}$, define the informal metric tensor

$$g_h(\dot h, \dot h) := \inf_j \left\{ \int_0^1 \frac{j^2}{M(h)} \,\mathrm{d}x : \ \partial_x j + \dot h = 0 \right\}.$$

Euler-Lagrange gives

$$g_h(\dot h, \dot h) = \int_0^1 M(h)(\partial_x f)^2 \,\mathrm{d}x, \qquad \dot h + \partial_x(M(h)\partial_x f) = 0.$$

With $G(h)$ denoting the inverse of $G^{-1}(h)$ on zero-mean functions,

$$g_h(\dot h, \dot h) = \int_0^1 \dot h \, G(h) \dot h \,\mathrm{d}x = \|\dot h\|^2_{H^{-1}_{M(h)}}.$$

For general M this is an informal geometry; for concave M it can be made rigorous *[Dolbeault–Nazaret–Savaré, 2009]*.

With these choices

$$\partial_t h = -\partial_x \Big(M(h) \partial_{xxx} h \Big) = -\nabla_{\mathcal{M}} \mathcal{E}(h).$$

Limitations of the deterministic thin film equation

In thin films thermal fluctuations are relevant: Hydrodynamic description possibly not justified and thermal fluctuations are present at small scales. [Davidovitch, Moro, Stone; Phys. Rev. Let. 2005]

Speed of front propagation (Tanner's law):

Conjecture: For

$$\partial_t h = -\partial_x (h^m \partial_{xxx} h),$$

with $m \geq 3$ the free interface $\partial\{h(t) > 0\}$ is constant.

Based on the non-existence of self-similar solutions for $m \geq 3$.

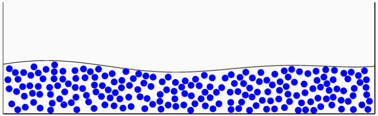


FIG. 1. *A thin liquid film consisting only of a limited number of fluid molecules.*

(source: Fischer, Grün 2018)

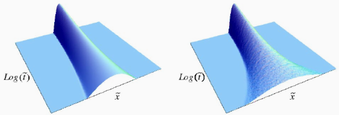


FIG. 2 (color online). Average shape of the droplet $\langle \tilde{h}(\tilde{x}, \tilde{t}) \rangle$ over 50 realizations as a function of time for zero temperature (left) and $\sigma = 10^{-2}$ (right). The right picture clearly shows the enhanced spreading of the droplet in the presence of thermal fluctuations. The numerical parameters used in this simulation are $\Delta\tilde{t} = 0.01$, $\Delta\tilde{x} = 0.05$, and $\tilde{b} = 0.01$.

(source: Davidovitch, Moro, Stone 2005)

Rupture time scales [Grün, Mecke, Rauscher; J. Stat. Phys. 2006], [Nesic, Cuerno, Moro, Kondic; 2017]

Figure 2: Snapshots at times $t = 10, 12, 13, 14, 15, 15.5, 15.75, 16$ for the deterministic thin-film equation. Discretisation parameters are the grid spacing $a = 2^{-9}\,L$ and time step $\tau = a^{\frac{5}{2}}$. (source: Grün, Mecke, Rauscher 2006)

Experiments: Deterministic thin film predicts the quotient

$$\frac{\text{rupture time-scale}}{\text{droplet-formation time-scale}}$$

too large compared to experiments.

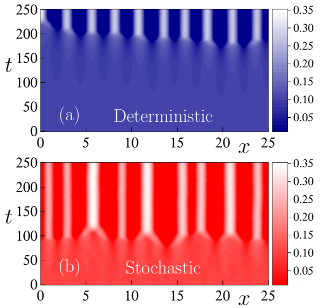


FIG. 1. Space-time plot of droplet formation and evolution as predicted by Eq. (1) for $\sigma = 0$ (a) and $\sigma = 10^{-2}$ (b), for the same parameter values and initial conditions, see main text. Brighter (darker) color corresponds to larger (smaller) values of the film thickness $h(x,t)$.

Derivation of the stochastic thin film equation

1. Derivation from stochastic Navier-Stokes
2. Gradient flow structure and fluctuation-dissipation principle

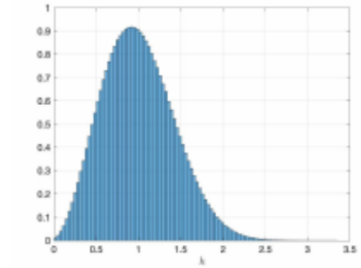
Equilibrium: Gibbs measure and Brownian excursion

Recall: $\partial_t h = -\partial_x\Big(M(h)\partial_{xxx} h\Big) = -\nabla_{\mathcal{M}}\mathcal{E}(h)$.
The formal equilibrium invariant Gibbs measure is

$$\nu(\,\mathrm{d}h) = \frac{1}{Z} e^{-\beta\mathcal{E}(h)}\,\mathrm{d}h,$$

where β is inverse temperature. The corresponding Gaussian free field is

$$\mu = \frac{1}{Z}\exp\left(-\frac{\beta}{2}\int_0^1 (\partial_x h)^2\,\mathrm{d}x\right)\,\mathrm{d}h.$$



Plot $h(x)$ under ν

Here we condition on non-negative and normalized functions:

$$\nu(\,\mathrm{d}h) = \frac{1}{Z}\mathbf{1}_{\{h\geq 0\}}\,\mathrm{d}\mu(h),$$

interpreted as a **conservative Brownian excursion**, with μ the Gaussian free field centered at 1.

Note: Due to entropic repulsion ν is concentrated on strictly positive functions.

Variational Fokker–Planck dynamics: Want ν to be reversible invariant for the stochastic thin-film dynamics. Let $f_t = \frac{\mathrm{d}\nu_t}{\mathrm{d}\nu}$. The time evolution is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{M}} \zeta f_t \,\mathrm{d}\nu = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{M}} \zeta \,\mathrm{d}\nu_t = -\frac{1}{\beta}\int_{\mathcal{M}} g_h(\nabla\zeta(h), \nabla f_t(h))\,\mathrm{d}\nu(h) = -\frac{1}{\beta}\mathcal{D}(\zeta, f_t).$$

- Integration by parts against ν produces the gradient-flow drift.
- The second-order term is the diffusion induced by thermal fluctuations.
- Symmetry of g gives a symmetric $L^2(\mathrm{d}\nu)$ generator, hence reversibility.

On the level of SPDE this (**informally**) corresponds to the SPDE

$$\partial_t h = -\partial_x(M(h)\partial_{xxx} h) + \sqrt{\frac{2}{\beta}}\partial_x(M^{1/2}(h)\xi),$$

with ξ space-time white noise.

Singularity and renormalization: The stochastic thin-film equation is written formally as

$$\partial_t h + \partial_x(M(h)\partial_{xxx} h) = \sqrt{\frac{2}{\beta}}\partial_x(M^{1/2}(h)\xi),$$

where ξ is space-time white noise. The stochastic integral and the drift are singular:

$$h \in C^{1/2-}, \qquad M(h)\partial_{xxx} h = C^{1/2-} \times C^{-5/2-},$$

$$M^{1/2}(h)\xi = C^{1/2-} \times C^{-5/2-}.$$

Thus a renormalization is expected. Choice of discretization crucial!

Regularity structures: Gvalani–Tempelmayr (2023)

Conformal Galerkin discretization

Fix $N \in \mathbb{N}$ and an equidistant partition of the torus $\{x_i\}$. Use continuous, piecewise-linear finite elements:

$$\mathcal{M}_N := \left\{ h : \begin{array}{l} h \text{ is 1-periodic, piecewise linear, continuous,} \\ h > 0, \quad \displaystyle\int_0^1 h \, \mathrm{d}x = 1 \end{array} \right\},$$

with $T\mathcal{M}_N$ defined analogously. The energy is restricted conformally:

$$\mathcal{E}_N := \mathcal{E}|_{\mathcal{M}_N}.$$

This yields a measure ν_N on $\mathcal{M}_N$.

How to discretize the geometry/mobility?

$$g_h(\dot{h}, \dot{h}) := \inf_j \left\{ \int_0^1 \frac{j^2}{M(h)} \, \mathrm{d}x : \ \partial_x j + \dot{h} = 0 \right\}.$$

Caution: The simple restriction of g to $T\mathcal{M}_N$ is not the right discrete geometry.

Conformal mixed finite elements with mass lumping: For $\dot{h}$ piecewise linear, set

$$g_h^N(\dot{h},\dot{h}) := \inf_j \left\{ \int \frac{j^2}{M(h)}\,\mathrm{d}x : \ j \text{ piecewise constant}, \ \int j \partial_x \zeta \,\mathrm{d}x = \frac{1}{N}\sum_i \dot{h}_i \zeta_i \right\}.$$

Conclusion: Discretized Dirichlet form $\mathcal{D}^N(\zeta, f_t) = \int_{\mathcal{M}^N} g_h^N(\nabla\zeta(h), \nabla f_t(h))\,\mathrm{d}\nu^N(h)$.

This corresponds to discrete mobility

$$M_\alpha^N(h) := \left(\fint_{I_\alpha} \frac{1}{M(h(x))}\,dx \right)^{-1}.$$

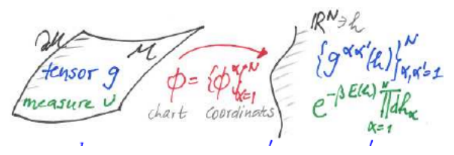
Entropic consistency: preserve the mathematical entropy dissipation. For the deterministic equation

$$\partial_t h = -\partial_x(M(h)\partial_{xxx} h),$$

the entropy $S(h) = \int s(h)\,\mathrm{d}x$, $s''(h) = \frac{1}{M(h)}$ is Lyapunov and satisfies: $\frac{\mathrm{d}}{\mathrm{d}t} S(h) = -\int (\partial_{xx} h)^2\,\mathrm{d}x$. Grün–Rumpf preserve this structure by enforcing the chain rule on the discrete level.

Charts:

$$(\varphi^\alpha) : \mathcal{M}_N \to \mathcal{U}_N.$$



Gives rise to matrix $(g_{\alpha\alpha'})_{\alpha,\alpha'}$, i.e. discrete metric tensor in coordinates and its inverse

$$g^{\alpha\alpha'}(h) = g^h\Big(\operatorname{diff}\varphi^\alpha\big|_h, \operatorname{diff}\varphi^{\alpha'}\Big|_h\Big)$$

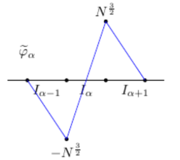


FIGURE 3. An element $\widetilde{\varphi}_\alpha$ of the *zigzag basis*

E.g., zigzag basis

$$\mathcal{U}_N := \{z \in \mathbb{R}^N : \sum_{\alpha=1}^N z^\alpha = 0, \quad 1+\sqrt{N}\,(A^T z)^i > 0 \text{ for all } i = 1, \dots, N\}.$$

Avantage: discrete metric tensor diagonalizes

$$g_{\alpha\alpha'} = \int_{I_\alpha} \frac{1}{M(h)}\,dx\,\delta_{\alpha\alpha'}, \qquad g^{\alpha\alpha'}(h) = \left(\int_{I_\alpha} \frac{1}{M(h)}\,dx\right)^{-1} \delta^{\alpha\alpha'}.$$

On $\mathcal{U}_N$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{U}_N} \zeta \,\mathrm{d}\nu_{t,N} = -\frac{1}{\beta} \int_{\mathcal{U}_N} g^{\alpha\alpha'} \partial_\alpha \zeta\, \partial_{\alpha'} f_t \,\mathrm{d}\nu_N.$$

Itô form: For $\rho_t = f_t \,\mathrm{d}\nu / \mathrm{d}h$,

$$\partial_t \rho = \partial_\alpha \underbrace{\left(g^{\alpha\alpha'} \left(\frac{1}{\beta}\partial_{\alpha'}\rho_t + \rho_t \partial_{\alpha'} E\right)\right)}_{J} \quad \text{in } \mathcal{U}_N,$$

with reflecting boundary conditions.Later: $m \geq 1$, the boundary is inaccessible, so the reflecting condition is inactive and need not be imposed.

Detailed balance: $J(\mathrm{d}\nu/\mathrm{d}h) = 0$ for $\mathrm{d}\nu/\mathrm{d}h = e^{-\beta E(h)}$.

Writing the Fokker–Planck equation in Itô form gives

$$\mathrm{d}h_t^\alpha = \left(-g^{\alpha\alpha'}\partial_{\alpha'}E(h_t) + \frac{1}{\beta}\partial_{\alpha'}g^{\alpha\alpha'}(h_t)\right)\mathrm{d}t + \sigma^\alpha_{\alpha'}(h_t)\sqrt{\frac{2}{\beta}}\,\mathrm{d}W_t^{\alpha'},$$

with reflecting boundary conditions, where $g^{\alpha\alpha'} = \sum_{\alpha''}\sigma^\alpha_{\alpha''}\sigma^{\alpha'}_{\alpha''}$

Key point: The Itô correction $\frac{1}{\beta}\partial_{\alpha'}g^{\alpha\alpha'}$ is required by detailed balance.

Correction term and continuum analogues: With nodal hat basis coordinates

$$(\varphi^i) : \mathcal{M}_N \to \Delta_N,$$

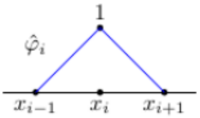


FIGURE 1. An element $\hat{\varphi}^i$ of the hat basis

the dynamics becomes

$$\mathrm{d}h_t = \left(-A^T G^{-1}(h_t) A A^T A h_t + \frac{N}{\beta} A^T \bar{D} \cdot G^{-1}(h_t)\right) \mathrm{d}t + A^T \sqrt{G^{-1}(h_t)} \sqrt{\frac{2N}{\beta}}\, \mathrm{d}W_t.$$

The correction term satisfies, formally,

$$\frac{N}{\beta} A^T \bar{D} \cdot G^{-1}(h_t) \longrightarrow -\frac{N}{\beta} \partial_x \left(M(h)^2 \partial_x \frac{M'(h)}{M(h)^2} \right).$$

For $M(h) = h^m$ this is

$$c_m \frac{N}{\beta} \partial_x \big(h^{m-2} \partial_x h \big).$$

Strict positivity via stochastic entropy: Let

$$S(h) := \frac{1}{N}\sum_{i=1}^{N} s(h_i), \qquad s''(h) = \frac{1}{M(h)}.$$

The Grün–Rumpf discretization satisfies the discrete chain rule.

Theorem

Let h_0 satisfy $\mathbb{E}[S(h_0)] < \infty$ and $M(h) \sim h^m$, $m \geq 3$[1]. Then

$$\mathbb{E}[S(h_t)] + \int_0^t \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N}\Big((A^T A h_r)_i\Big)^2\right] \mathrm{d}r = \mathbb{E}[S(h_0)] + \frac{2N^3}{\beta} t.$$

If $\inf_x h_0 > 0$ and $T < \infty$, then $\inf_{x,t\leq T} h_t > 0$ almost surely for $m \geq 3$.

Not a stable estimate for $N \to \infty$.

[1] [G., Otto, Sauerbrey 2026+: extension to $m \geq 2$ (sharp), and $m \geq 1$ on Dirichlet form level

Large deviations: The rate function for the stochastic thin-film equation is

$$I_T(h) := \frac{1}{2}\int_0^T g_{h_t}\left(\frac{\mathrm{d}h_t}{\mathrm{d}t} + \nabla E(h_t), \frac{\mathrm{d}h_t}{\mathrm{d}t} + \nabla E(h_t)\right)\,\mathrm{d}t.$$

For a solution h^β of the STFE, informally,

$$\mathbb{P}(h^\beta \approx h) \approx e^{-\beta I_T(h)}.$$

Theorem

Let $M(h) = h^m$, $T > 0$.

- *If $m < 8$, then there exists h with*

$$I_T(h) < \infty, \qquad \min_x h_0 > 0, \qquad \min_x h_T = 0.$$

- *If $m \geq 8$, and $h_0 \equiv 1$,*

$$I_T(h) \to \infty$$

as $\inf_x h_T \to 0$.

Comparison to prior discretizations: Prior works avoided the Itô correction term:

- Grün–Mecke–Rauscher et al.: keep positivity but lose reversibility, due to upwinding in the stochastic term
- Durán-Olivencia–Gvalani–Kalliadasis–Pavliotis: lose positivity but keep reversibility with central differences.
- Zhao–Liu–Lockerby–Sprittles (2022): nonuniform grids, higher-order finite differences, correlated noise.

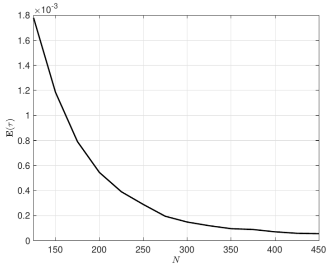
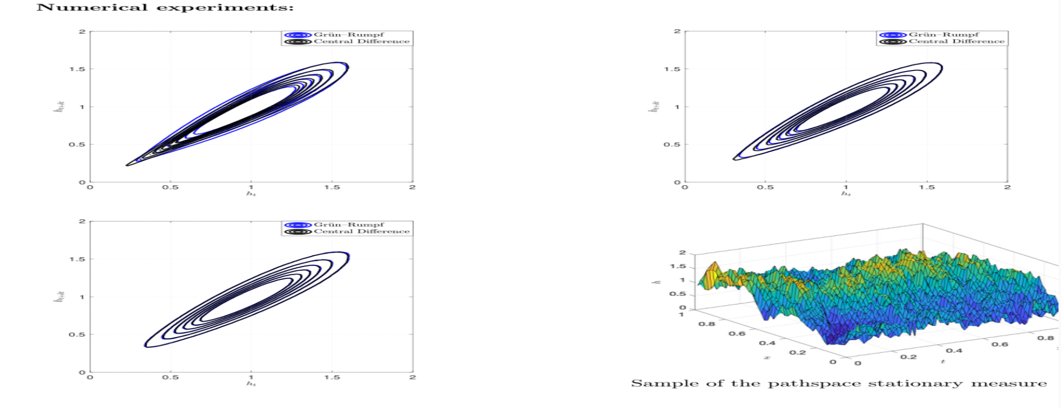


FIGURE 7. The dependence of the mean exit time of the central difference discretization on N. The simulations were performed with the following parameters: $\Delta t = 10^{-10}$, $\beta = 1$, $M = 100$, and $h_0 \equiv 1$.

This discretization: Keeps both positivity (due to mobility discretization) and reversibility (due to the correction term).



Phase-space comparisons of Grün–Rumpf and central-difference discretizations, and a sample of the path-space stationary measure.

Observation: In equilibrium, difference of different discretizations appears to decay in the limit

Takeaways:

- Conformal discretizaion unveils necessary Ito correction terms
- Geometric interpretation of the Grün–Rumpf mobility
- Strict positivity
- Continuum touch down

Literature:

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