Fractional time differential equation as a singular limit of the Kobayashi–Warren–Carter system

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Y. Giga, A. Kubo, H. Kuroda, J. Okamoto, K.S. and M. Uesaka.
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Kobayashi–Warren–Carter model

Grain boundary

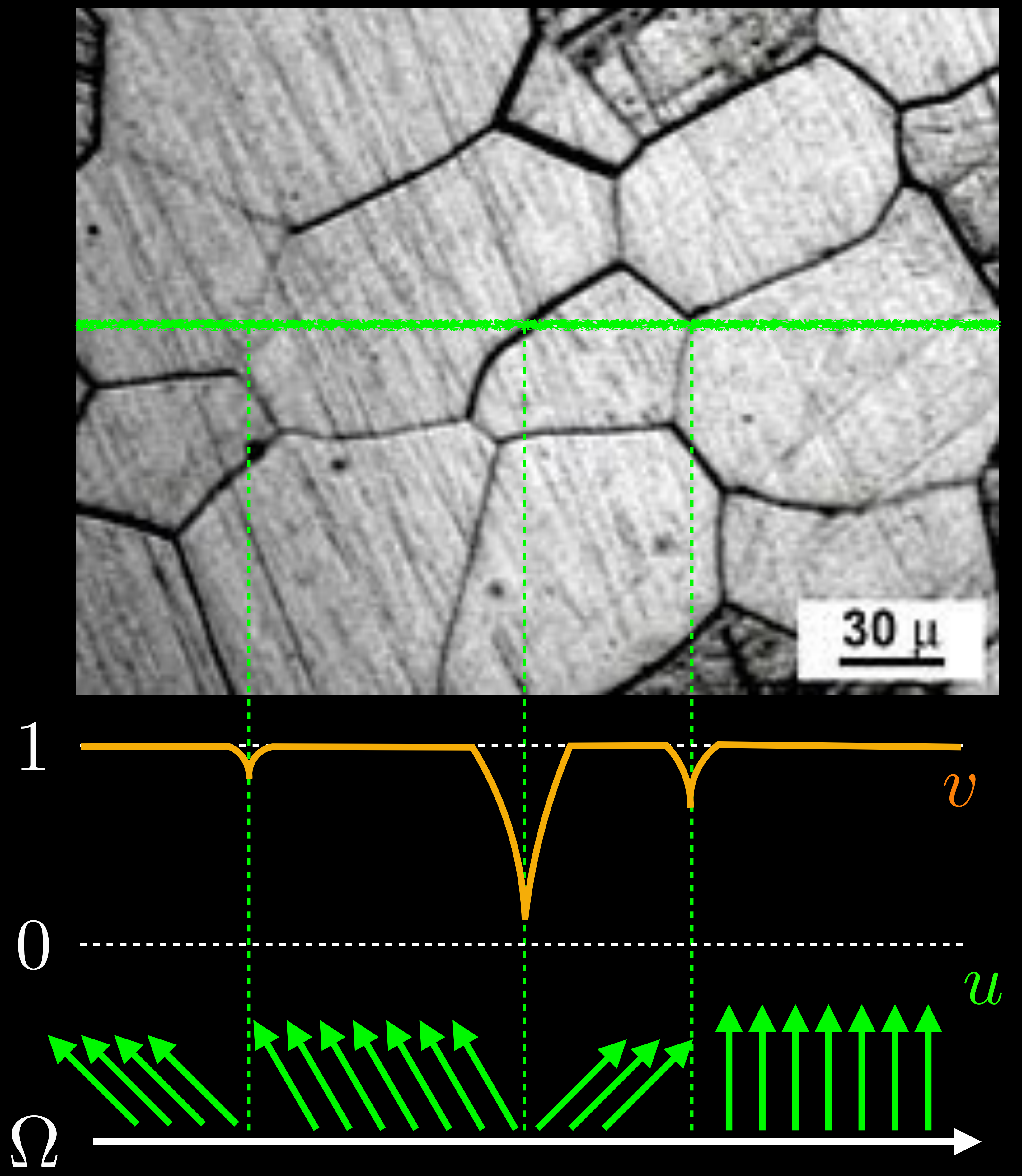
interface between crystallines in a polycrystalline material

Kobayashi–Warren–Carter (KWC) energy

$$E^{\varepsilon}_{\mathrm{KWC}}(u,v) := \int_{\Omega} \alpha_0(v)|\nabla u| + \underbrace{\int_{\Omega} \frac{\varepsilon}{2}|\nabla v|^2 \,\mathrm{d}x + \int_{\Omega} \frac{1}{2\varepsilon} F(v)\,\mathrm{d}x}_{=:\, E^{\varepsilon}_{\mathrm{sMM}}(v)}$$

$\alpha_0(v) \geq 0 \quad$ (e.g., $\alpha_0(v) = sv^2$)

$F(v)$: single-well potential (e.g., $F(v) = a^2(v-1)^2, \ a > 0$)



KWC model ⋯ (weighted) L^2-gradient flow of $E^{\varepsilon}_{\mathrm{KWC}}$

(Kobayashi–Warren–Carter ('00), Warren–Kobayashi–Carter ('00))

$$\alpha_w(v)u_t = \operatorname{div}\left(\alpha_0(v)\frac{\nabla u}{|\nabla u|}\right), \quad \tau v_t = \varepsilon \triangle v - \frac{1}{2\varepsilon}F'(v) - \alpha_0'(v)|\nabla u|$$

$$\tau_0(v^2+\delta)u_t = s\,\operatorname{div}\left((v^2+\delta')\frac{\nabla}{|\nabla u|} + \mu \nabla u\right)$$

Ito–Kemmochi–Yamazaki ('09, '09, '12)
Moll–Shirakawa ('14), Moll–Shirakawa–Watanabe ('17)
Shirakawa–Watanabe ('13, '14)

★ Singular limit of the KWC problem as $\varepsilon \searrow 0$

★ gradient flow of $E^{\varepsilon}_{\mathrm{KWC}} \xrightarrow[\varepsilon \searrow 0]{}$ gradient flow of E^{0}_{KWC}?

Giga–Okamoto–Uesaka ('23)
Giga–Okamoto–S.–Uesaka (to appear)

Fractional time differential equation

Stationary solution

$F(v)=a^2(v-1)^2 \ (a\geq 0), \quad \alpha_0(v)=v^2$

$$\begin{cases} \tau v_t = \varepsilon\triangle v - \dfrac{1}{2\varepsilon}F'(v) - \alpha_0'(v)|\nabla u| & \text{in } I=(-L,L) \\ \alpha_w(v)u_t = \mathrm{div}\left(\alpha_0(v)\dfrac{\nabla u}{|\nabla u|}\right) & \text{in } I \qquad (*) \end{cases}$$

DBC for u : $u(-L,t)=0$, $u(L,t)=b>0$

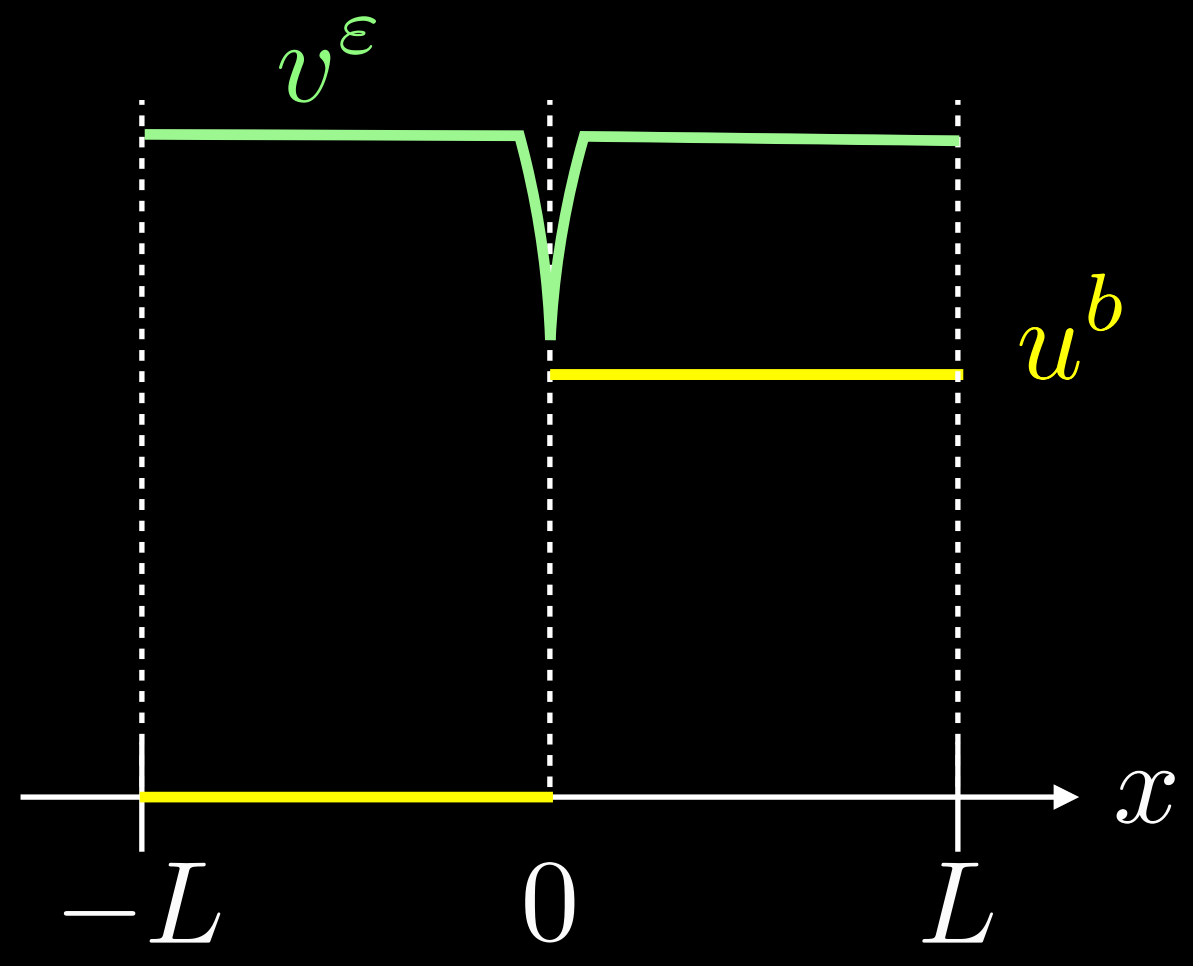
NBC for v : $v_x(\pm L,t)=0$

Lem. 1 (stationary solution) For $\beta\in C(\overline{I})$ satisfying $\beta(0)\leq\beta(x)$ $({}^\forall x\in I)$,

$$u^b(x) := \begin{cases} b & \text{for } x>0 \\ 0 & \text{for } x<0 \end{cases} \implies$$

u^b is a solution to

$$\begin{cases} \left(\beta\dfrac{u_x}{|u_x|}\right)_x = 0 & \text{in } I \\ u(-L)=0, \quad u(L)=b \end{cases}$$



v_0^ε : even, non-decreasing, i.e., $v_{0,x}^\varepsilon(x)x\geq 0$ for $x\in(-L,L)$

$\rightsquigarrow$ u^b : stationary solution to $(*)$ under DBC

$$\begin{cases} \dfrac{\tau_1}{\varepsilon}v_t = \varepsilon v_{xx} - \dfrac{a^2(v-1)}{\varepsilon} - 2bv\partial_x(1_{x>0}) & \text{in } I\times(0,\infty) \\ v_x(\pm L,t)=0 & \text{for } t>0 \\ v(x,0)=v_0^\varepsilon(x) & \text{for } x\in\Omega \end{cases}$$

$y=\dfrac{x}{\varepsilon}, \ V=V^\varepsilon(y,t):=v^\varepsilon(\varepsilon y,t)$

$$\tau_1 V_t = V_{yy} - a^2(V-1) - 2bV\partial_y(1_{y>0})$$

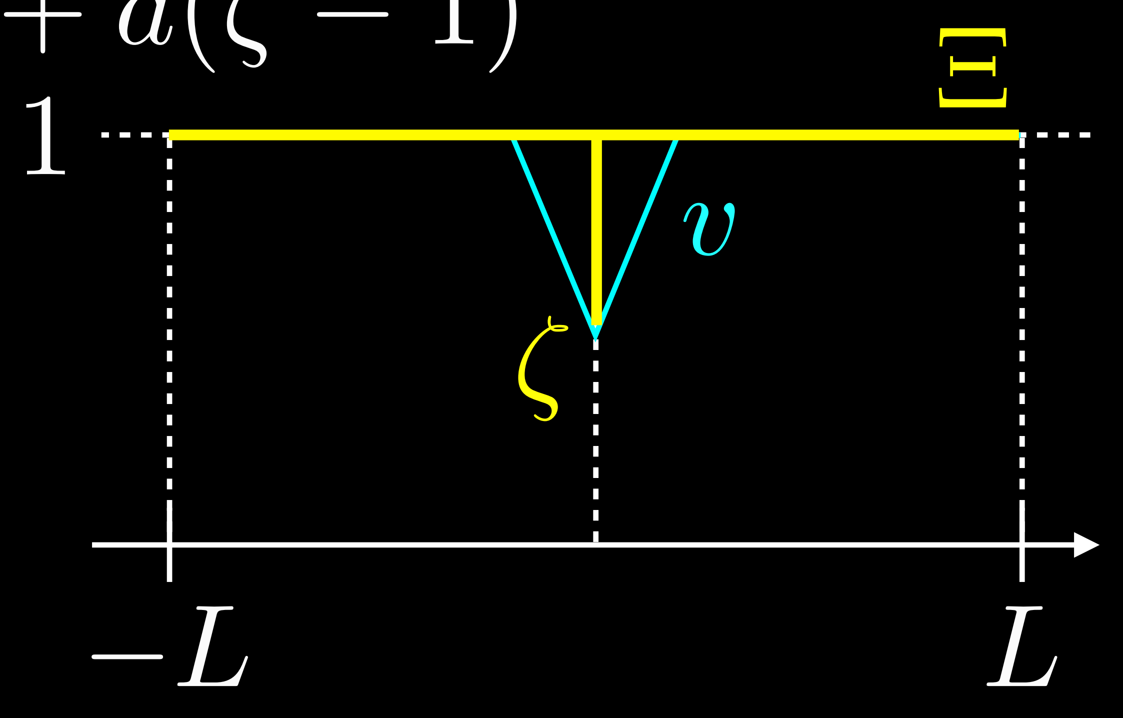
in $(-L/\varepsilon, L/\varepsilon)\times(0,\infty)$

✔ Equation which $\xi := \lim_{\varepsilon\searrow 0} v^\varepsilon(0,t)$ solves

 Giga–Okamoto–Uesaka ('23)

$$E^{\varepsilon}_{\mathrm{sMM}}(v) = \int_I \frac{\varepsilon}{2}|\nabla v|^2\,\mathrm{d}x + \int_I \frac{1}{2\varepsilon}F(v)\,\mathrm{d}x \xrightarrow[\Gamma]{} E^{0}_{\mathrm{sMM}}(\zeta) = b\zeta^2 + 2G(\zeta) = b\zeta^2 + a(\zeta-1)^2$$

$$\text{if} \quad v \xrightarrow[\mathrm{g}]{} \Xi, \quad \Xi(x) := \begin{cases} \{1\} & \text{for } x \neq 0, \\ [\zeta, 1] & \text{for } x = 0, \end{cases} \qquad \zeta \in (0,1)$$



Lem. 2 (Singular limit equation)

V : bounded sol. to

$$\begin{cases} \tau_1 V_t = V_{yy} - a^2(V-1) - 2bV\partial_y(1_{y>0}) & \text{in } \mathbb{R}\times(0,\infty) \\ V(y,0) = 1 - c\mathrm{e}^{-a|y|} \quad (c\in\mathbb{R}) \end{cases}$$

well-prepared initial data, i.e., continuous & solves PDE outside $y=0$

$\Longrightarrow \quad \xi(t) := V(0,t)$ solves

$$\int_0^t m_a(t-s)\xi_s(s)\,\mathrm{d}s = -\operatorname{grad} E^{0,b}_{\mathrm{sMM}}(\xi)$$

where

$$m_a(t) := 2\left(f^{a^2}_{1/2}(t) + a^2\int_0^t f^{a^2}_{1/2}(s)\,\mathrm{d}s - a\right), \quad f^{\alpha}_{\beta}(t) := \frac{\mathrm{e}^{-\alpha t}t^{\beta-1}}{\Gamma(\beta)}$$

$$a = 0 \quad \rightsquigarrow \quad m_a(t) = 2f^{0}_{1/2}(t) = \frac{2}{t^{1/2}\sqrt{\pi}} \quad \rightsquigarrow \quad \text{(LHS) = Caputo derivative } \partial_t^{1/2}$$

Singular limit equation: sketch of the proof

$$w := V - 1 \;\; (w(x,0) = w_0(x) = -c\mathrm{e}^{-a|x|})$$

$$V_t = V_{yy} - a^2(V-1) - 2bV\partial_y(1_{y>0}) \quad \rightsquigarrow \quad w_t - w_{xx} + a^2 w + 2b(w+1)\delta = 0$$

$$\lambda\hat{w} - w_0 - \hat{w}_{xx} + a^2\hat{w} + 2b(\hat{w} + \lambda^{-1})\delta = 0 \qquad \hat{w}(x,\lambda) := \mathcal{L}[w](x,\lambda) := \int_0^\infty \mathrm{e}^{-\lambda t} w(x,t)\,\mathrm{d}t$$

$$\hat{w} = A\mathrm{e}^{-\sqrt{\lambda+a^2}|x|} - \frac{c}{\lambda}\mathrm{e}^{-a|x|} \longrightarrow A = \frac{-b(1-c)+ca}{\lambda(\sqrt{\lambda+a^2}+b)}$$

$$\eta(t) := w(0,t) \quad \rightsquigarrow \quad \hat{\eta}(\lambda) = \frac{ca+bc-b}{\lambda(\sqrt{\lambda+a^2}+b)} - \frac{c}{\lambda}$$

$$\rightsquigarrow \quad 2\left(\frac{\sqrt{\lambda+a^2}-a}{\lambda}\right)\hat{\eta}_t = -2(b+a)\hat{\eta} - 2b\hat{1} = -\mathcal{L}[\mathrm{grad}\, E^{0,b}_{\mathrm{sMM}}(\xi)]$$

$$\hat{m}_a(\lambda) = 2\left(\frac{\sqrt{\lambda+a^2}-a}{\lambda}\right)$$

Lem 2' V : bounded sol., $V(y,0) = 1 + w_0$, w_0 : bounded & Lipschitz

$\Longrightarrow$ $\xi(t) := V(0,t)$ solves

$$m_a * \xi_t + m_a(\xi(0)-1) - \mathcal{L}^{-1}\left[2\sqrt{\lambda+a^2}\,g^a(\lambda,w_0)\right] = -\,\mathrm{grad}\, E^{0,b}_{\mathrm{sMM}}(\xi)$$

$$\text{where} \quad g^a(\lambda,w_0) := (G^a_\lambda *_x w_0)(0), \quad G^a_\lambda(y) := \frac{\mathrm{e}^{-\sqrt{\lambda+a^2}|y|}}{2\sqrt{\lambda+a^2}}$$

Convergence

Lem 3

V : bounded sol. to $\begin{cases} \tau_1 V_t = V_{yy} - a^2(V-1) - 2bV\partial_y(1_{y>0}) & \text{in } \mathbb{R}\times(0,\infty) \\ V_0 \ : \text{bounded \& unifformly continuous on } \mathbb{R} \end{cases}$

v^ε : sol. to $\begin{cases} \dfrac{\tau_1}{\varepsilon} v_t = \varepsilon v_{xx} - \dfrac{a^2(v-1)}{\varepsilon} - 2bv^\varepsilon \partial_x(1_{x>0}) & \text{in } I\times(0,\infty) \\ v_x(\pm L, t) = 0 \ (t>0), \quad v(x,0) = v_0^\varepsilon(x) \end{cases}$

$y = \dfrac{x}{\varepsilon}$

$V = V^\varepsilon(y,t) = v^\varepsilon(\varepsilon y, t)$

$$\lim_{\varepsilon \searrow 0} \sup_{|y|\le L/\varepsilon} |V_0^\varepsilon(y) - V_0(y)| = 0, \quad V_0^\varepsilon := V^\varepsilon|_{t=0} \in C[-L/\varepsilon, L/\varepsilon]$$

$\Longrightarrow$ $V^\varepsilon \longrightarrow V$ locally uniformly in $\mathbb{R}\times[0,\infty)$

$\xi^\varepsilon(t) := v^\varepsilon(0,t) = V^\varepsilon(0,t) \longrightarrow \xi(t) := V(0,t)$ locally uniformly in $[0,\infty)$

$$\lim_{|y|\to 0} (V_0(y)-1)|y| = 0 \implies \lim_{\varepsilon\searrow 0} \sup_{0\le t\le T} \|V^\varepsilon - V\|_{L^\infty(I_\varepsilon)} = 0, \quad \lim_{|y|\to\infty} \sup_{0\le t\le T} (|V(y,t)-1||y|) = 0$$

Strategy of proof V_0^ε on I_ε $\rightsquigarrow$ $\overline{V_0^\varepsilon}$ on $\mathbb{R}$ $\rightsquigarrow$ $V_{0,\delta}^\varepsilon := \overline{V_0^\varepsilon} * \rho_\delta$, W_δ^ε : sol.

Arzelà–Ascoli theorem & diagonal argument $\rightsquigarrow$ convergent subsequence $\longrightarrow V$

V_0^ε
- odd part $\rightsquigarrow$ the problem without the term $V\partial_y(1_{y>0})$
- even part $\rightsquigarrow$ Robin boundary value problem

Convergence & Numerical results

Thm

v^ε : sol. to $\begin{cases} \frac{\tau_1}{\varepsilon} v_t = \varepsilon v_{xx} - \frac{a^2(v-1)}{\varepsilon} - 2bv^\varepsilon \partial_x (1_{x>0}) & \text{in } I \times (0,\infty) \\ v_x(\pm L, t) = 0 \ (t>0), \quad v(x,0) = v_0^\varepsilon(x) \end{cases}$

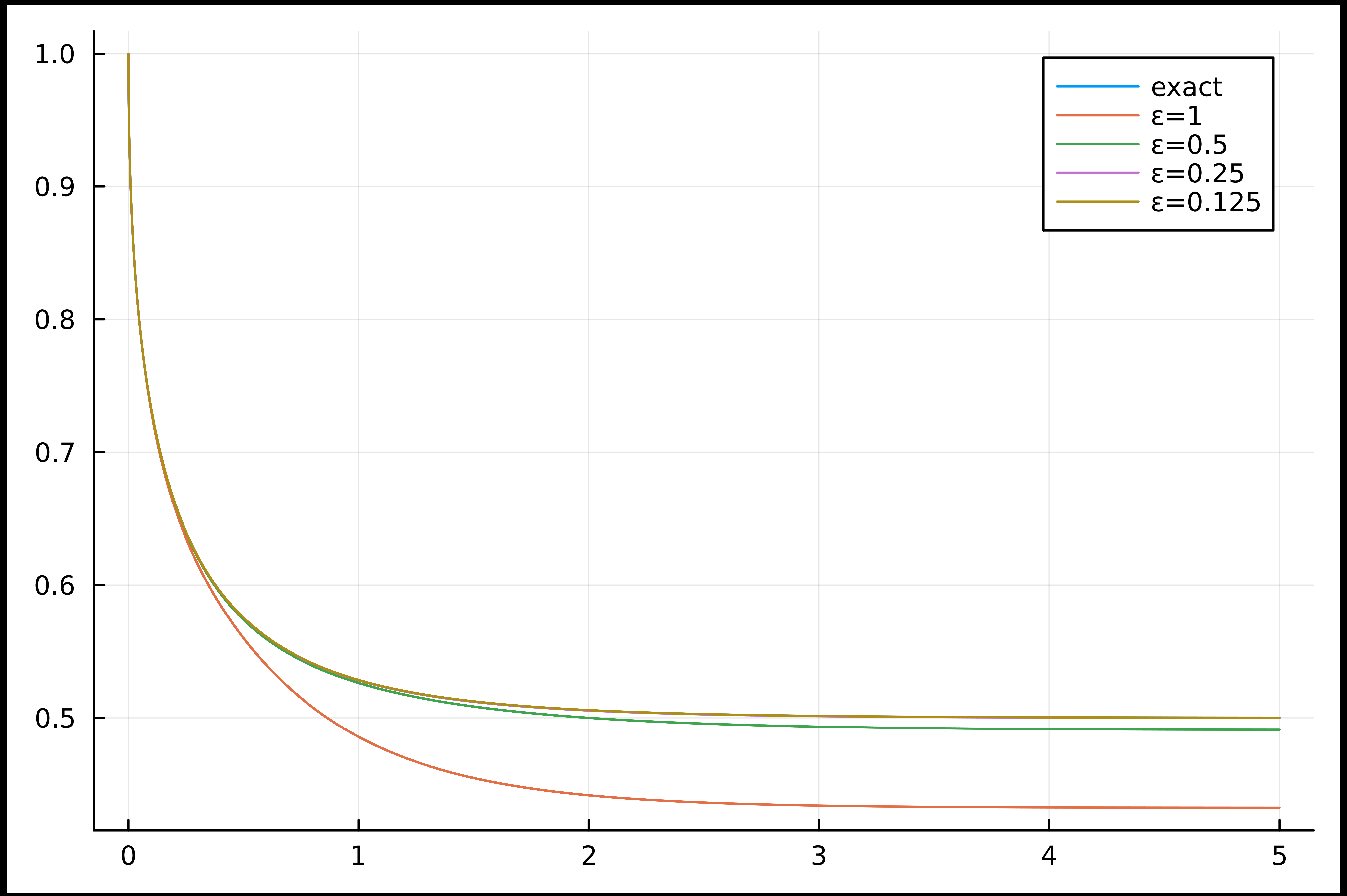
v_0^ε : well-prepared, i.e., $\sup_{x \in I} |v_0^\varepsilon(x) - (1 - ce^{-a|x|/\varepsilon})| \longrightarrow 0 \quad (\varepsilon \searrow 0)$

$\Longrightarrow$ $\xi^\varepsilon(t) \xrightarrow[\varepsilon \searrow 0]{} \xi(t)$ locally uniformly in $[0,\infty)$, $\int_0^t m_a(t-s)\xi_s(s)\,\mathrm{d}s = -\operatorname{grad} E^{0,b}_{\mathrm{sMM}}(\xi)$

$v^\varepsilon \xrightarrow[\varepsilon \searrow 0]{} \Xi, \quad \Xi(x,t) := \begin{cases} \{1\} & \text{for } x \neq 0, \\ \text{close interval between } \xi(t) \text{ and } 1 & \text{for } x = 0 \end{cases}$

v_0 : even

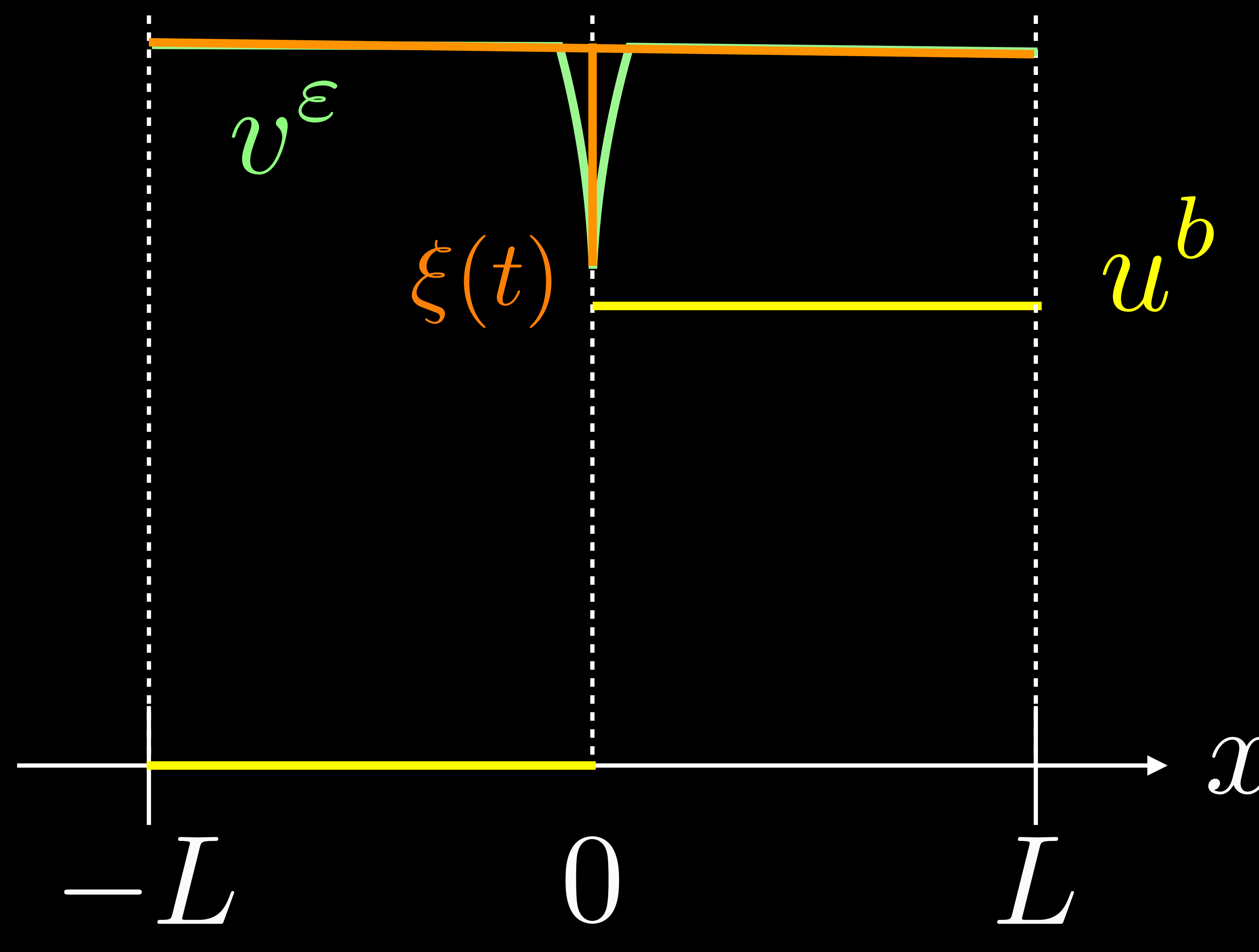
$$\begin{cases} \frac{\tau_1}{\varepsilon} v_t = \varepsilon v_{xx} - \frac{a^2(v-1)}{\varepsilon} & \text{in } (0,L)\times(0,\infty) \\ -v_x(0,t) + \frac{b}{\varepsilon} v(0,t) = 0 & \text{for } t>0 \\ v_x(L,t) = 0 & \text{for } t>0 \\ v(x,0) = v_0(x) \end{cases}$$



Summary

Kobayashi–Warren–Carter model

$$\begin{cases} \tau v_t = \varepsilon \triangle v - \dfrac{1}{2\varepsilon} F'(v) - \alpha_0'(v)|\nabla u| & \text{in } I \\ \alpha_w(v) u_t = \operatorname{div}\left(\alpha_0(v)\dfrac{\nabla u}{|\nabla u|}\right) & \text{in } I \end{cases}$$



$\downarrow$ $u = u^b$

$$\begin{cases} \dfrac{\tau_1}{\varepsilon} v_t^\varepsilon = \varepsilon v_{xx}^\varepsilon - \dfrac{a^2(v^\varepsilon - 1)}{\varepsilon} - 2bv^\varepsilon \partial_x(1_{x>0}) & \text{in } I \times (0,\infty) \\ v_x^\varepsilon(\pm L, t) = 0 \ (t > 0), \quad v^\varepsilon(x,0) = v_0^\varepsilon(x) \end{cases}$$

$$\xi^\varepsilon(t) := v^\varepsilon(0,t) \xrightarrow[\varepsilon \searrow 0]{} \xi(t), \quad \int_0^t m_a(t-s)\xi_s(s)\,\mathrm{d}s = -\operatorname{grad} E_{\mathrm{sMM}}^{0,b}(\xi)$$

$$E_{\mathrm{KWC}}^{\varepsilon,\lambda}(u,v;g) := \int_\Omega \alpha_0(v)|\nabla u| + \int_\Omega \frac{\varepsilon}{2}|\nabla v|^2\,\mathrm{d}x + \int_\Omega \frac{1}{2\varepsilon}F(v)\,\mathrm{d}x + \frac{\lambda}{2}\int_\Omega (u-g)^2\,\mathrm{d}x$$

Thank you for your attention!