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Remark on boundary conditions for the KPZ equation

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The Kardar-Parisi-Zhang (KPZ) equation

$$\frac{\partial h}{\partial t} = \frac{c}{2} \cdot (\nabla h)^2 + \nu \cdot \Delta h$$

Kardar M, Parisi G and Zhang Y C 1986 Phys. Rev. Lett. 56 889.

$h(x, y, t)$ Is (reduced) height of a surface

c Is a rate of sputtering

ν Is a coefficient of a surface diffusion

$\vec{J} = -\nu \cdot \nabla h$ Is a flux of the surface diffusion

The KPZ equation ought to be provided by initial condition:

$$h(x, y, 0) = h_0(x, y)$$

As a rule the KPZ equation is solved on the whole plane:

$$(x, y) \in R^2$$

But in practice of microelectronics:

$$(x, y) \in D \subset R^2$$

The KPZ equation should be endowed by boundary conditions, for example:

$$\left. \frac{\partial h}{\partial n} \right|_{\partial D} = 0$$

The question is to compare solution of the Cauchy problem on the plane and solution of the mixed problem the KPZ equation with the following restriction:

$$diam(\text{sup } ph_0) \ll diam D$$

To clarify this question let one consider growing surfaces with cylindrical generatrix only

$$\frac{\partial h}{\partial t} = \frac{c}{2} \cdot \left(\frac{\partial h}{\partial x} \right)^2 + \nu \cdot \frac{\partial^2 h}{\partial x^2} \quad h(x,0) = h_0 \left(\frac{x}{l} \right)$$

Let us rescale variables as follows: $\frac{x}{l} \rightarrow x \quad \frac{\nu \cdot t}{l^2} \rightarrow t \quad \frac{c \cdot h}{\nu} \rightarrow h$

$$\frac{\partial h}{\partial t} = \frac{1}{2} \cdot \left(\frac{\partial h}{\partial x} \right)^2 + \frac{\partial^2 h}{\partial x^2} \quad h(x,0) = h_0(x)$$

Neumann boundary conditions: $\left. \frac{\partial h}{\partial x} \right|_{x=-L} = \left. \frac{\partial h}{\partial x} \right|_{x=+L} = 0$

Let one introduce new auxiliary function $\varphi(x,t)$: $h = 2 \cdot \ln \varphi$

$$\frac{\partial \varphi}{\partial t} = \frac{\partial^2 \varphi}{\partial x^2} \quad \varphi(x,0) = \exp\left[\frac{h_0(x)}{2}\right] \quad x \in R$$

$$\varphi(x,t) = \frac{1}{2\sqrt{\pi \cdot t}} \int_{-\infty}^{+\infty} \exp\left[-\frac{(x-\xi)^2}{4 \cdot t} + \frac{h_0(\xi)}{2}\right] \cdot d\xi$$

$$h_0(x) = 2 \cdot \ln[1 + m_0 \cdot \psi_0(x)] \quad 0 \leq \psi_0(x) \leq 1 \quad m_0 > -1$$

$$\varphi(x,t) = 1 + m_0 \cdot \psi(x,t) \quad \sup p \psi_0 = [-1,1]$$

$$\psi(x,t) = \frac{1}{2\sqrt{\pi \cdot t}} \int_{-\infty}^{+\infty} \exp\left[-\frac{(x-\xi)^2}{4 \cdot t}\right] \cdot \psi_0(\xi) \cdot d\xi$$

It is convenient to choose: $\psi_0(x) = \theta(1 - |x|)$

$\theta(z)$ is the Heaviside step function

$$\psi(x, t) = \frac{1}{2} \cdot \left[\operatorname{erf}\left(\frac{x+1}{2\sqrt{t}}\right) - \operatorname{erf}\left(\frac{x-1}{2\sqrt{t}}\right) \right]$$

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\zeta^2) \cdot d\zeta$$

is the Gauss error function

$$\psi_0(x) = (1 - |x|) \cdot \theta(1 - |x|)$$

$$\begin{aligned} \psi(x, t) = & \frac{1}{2} \cdot \left[\operatorname{erf}\left(\frac{x+1}{2\sqrt{t}}\right) - \operatorname{erf}\left(\frac{x-1}{2\sqrt{t}}\right) \right] + \\ & + \frac{x}{2} \cdot \left[\operatorname{erf}\left(\frac{x+1}{2\sqrt{t}}\right) - 2 \cdot \operatorname{erf}\left(\frac{x}{2\sqrt{t}}\right) + \operatorname{erf}\left(\frac{x-1}{2\sqrt{t}}\right) \right] + \\ & + \sqrt{\frac{t}{\pi}} \cdot \left[\exp\left(-\frac{(x+1)^2}{4 \cdot t}\right) - 2 \cdot \exp\left(-\frac{x^2}{4 \cdot t}\right) + \exp\left(-\frac{(x-1)^2}{4 \cdot t}\right) \right] \end{aligned}$$

$$h(x, t) = 2 \cdot \ln[1 + m_0 \cdot \psi(x, t)]$$

$$x \in [-L, L] \quad L \gg 1 \quad \frac{\partial \varphi}{\partial x} \Big|_{x=-L} = \frac{\partial \varphi}{\partial x} \Big|_{x=+L} = 0$$

$$\varphi(x, t) = 1 + m_0 \cdot \psi(x, t)$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2} \quad \psi(x, 0) = \psi_0(x) \quad \frac{\partial \psi}{\partial x} \Big|_{x=-L} = \frac{\partial \psi}{\partial x} \Big|_{x=+L} = 0$$

Separation of variables: $\psi(x, t) = \exp(-\lambda \cdot t) \cdot X(x)$

**Sturm-Liouville
problem:**

$$-X''(x) = \lambda \cdot X(x)$$

$$X'(-L) = X'(L) = 0$$

$$L^2([-L, L]) = V^+ \oplus V^-$$

$$\begin{array}{ccc}
\frac{1}{\sqrt{2L}} & \frac{1}{\sqrt{L}} \cdot \cos \frac{\pi \cdot n \cdot x}{L} & \frac{1}{\sqrt{L}} \cdot \sin \frac{\pi \cdot (2n-1) \cdot x}{2L} \\
\downarrow & \downarrow & \downarrow \\
\lambda_0 = 0 & \lambda_n^+ = \frac{\pi^2 n^2}{L^2} & \lambda_n^- = \frac{\pi^2 (2n-1)^2}{4L^2}
\end{array}$$

$$\psi_0(x) = \theta(1 - |x|)$$

$$\psi(x, t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} \exp\left(-\frac{\pi^2 n^2 t}{L^2}\right) \cdot \frac{\sin \pi n / L}{\pi n / L} \cdot \cos \frac{\pi \cdot n \cdot x}{L}$$

$$h(x, t) = 2 \cdot \ln[1 + m_0 \cdot \psi(x, t)]$$

$$\psi_0(x) = (1 - |x|) \cdot \theta(1 - |x|)$$

$$\psi(x, t) = \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} \exp\left(-\frac{\pi^2 n^2 t}{L^2}\right) \cdot \left(\frac{\sin \pi n / 2L}{\pi n / 2L}\right)^2 \cdot \cos \frac{\pi \cdot n \cdot x}{L}$$

$$h(x, t) = 2 \cdot \ln[1 + m_0 \cdot \psi(x, t)]$$

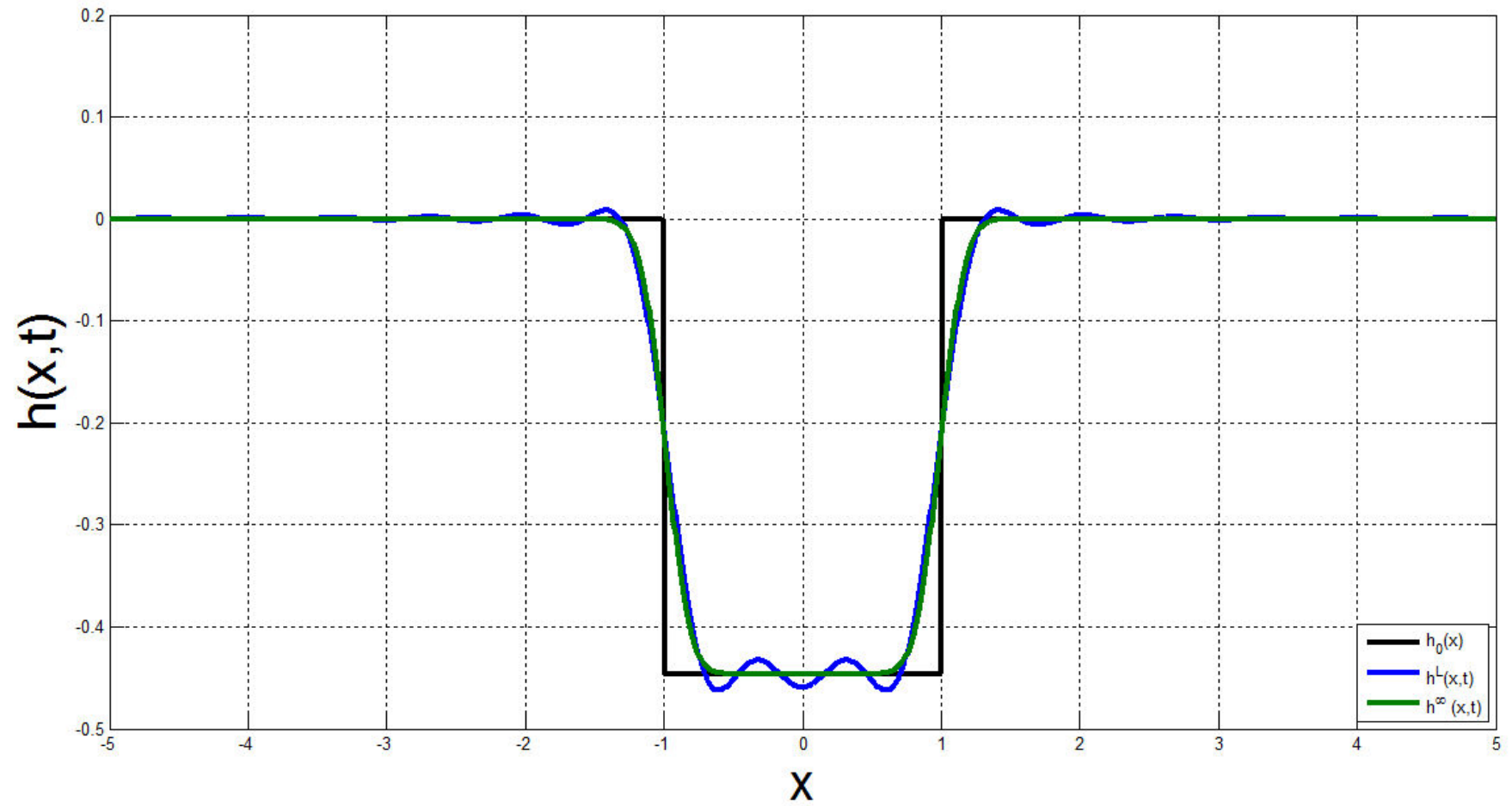
Results of computer experiment under values:

$$N = 30$$

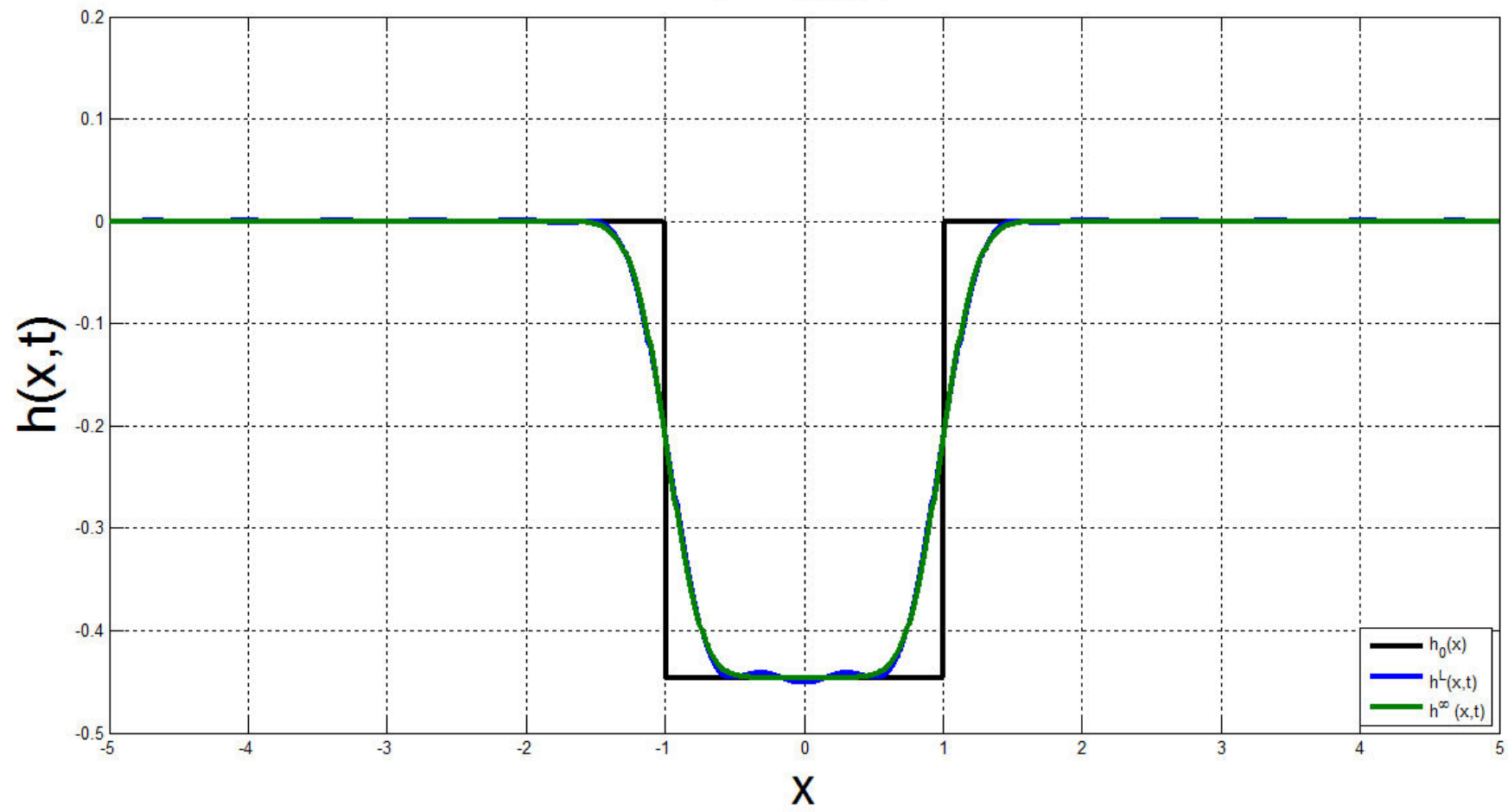
$$L = 10$$

$$m_0 = -0.2$$

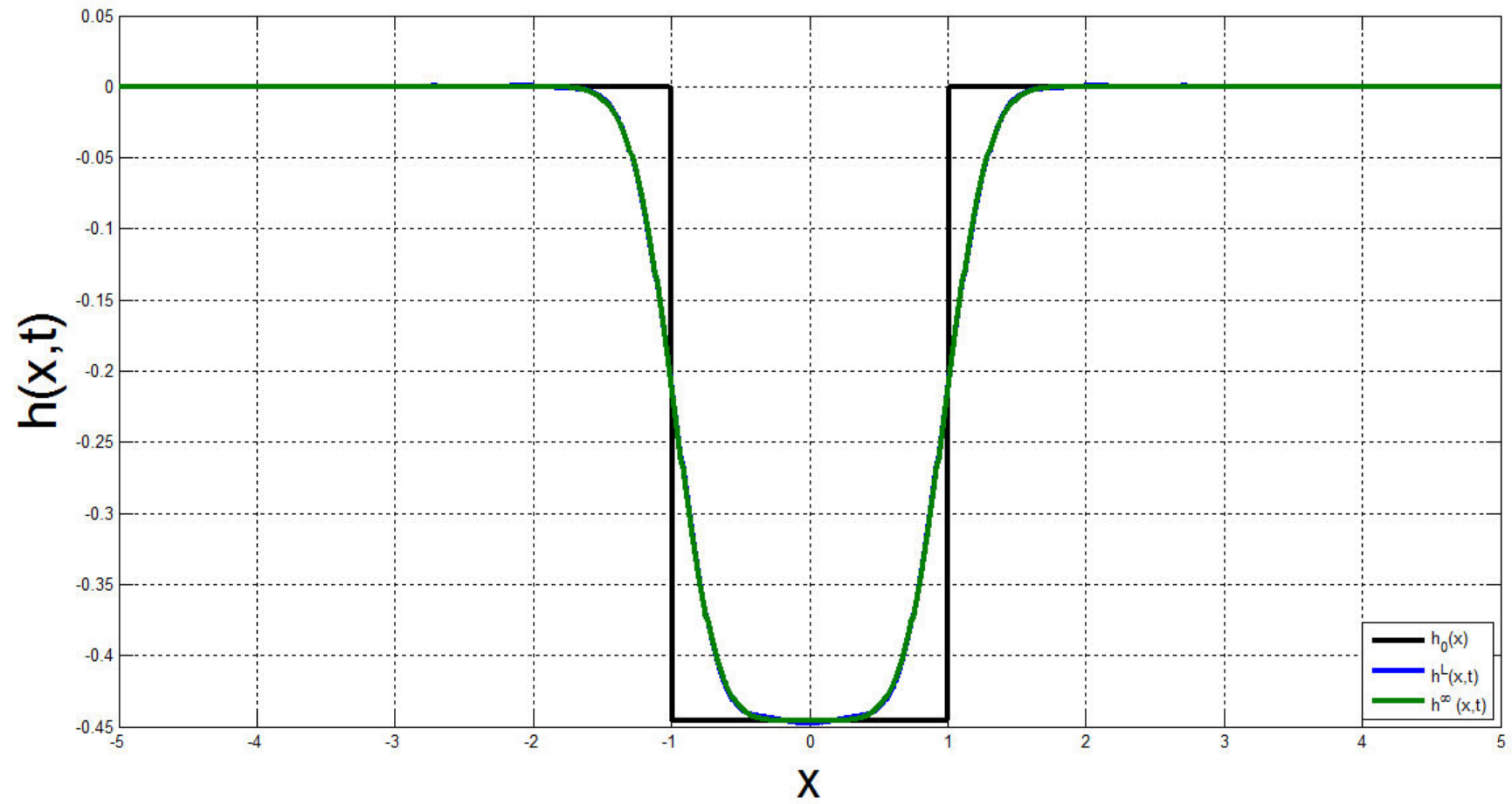
$t = 0.01$

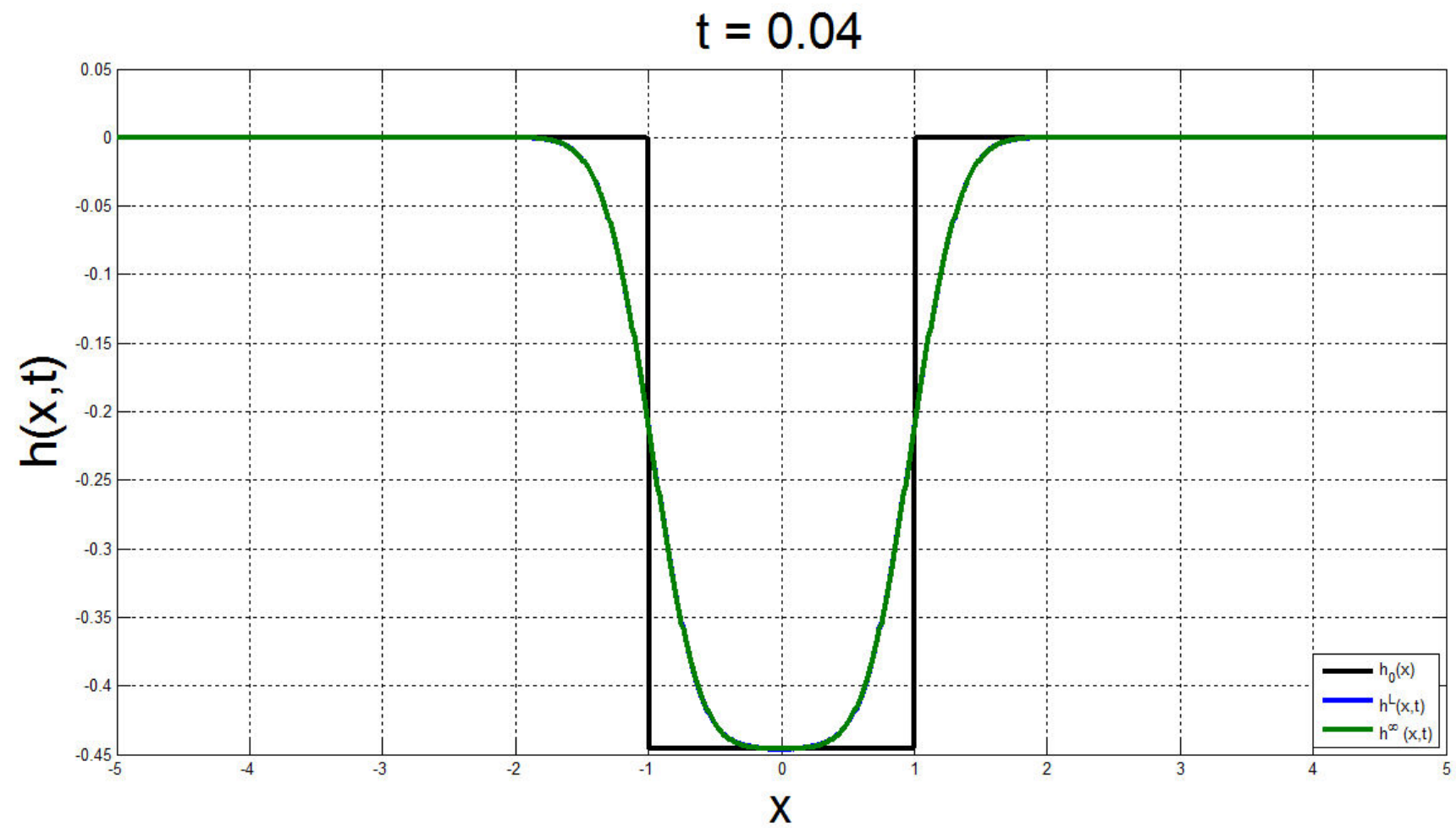


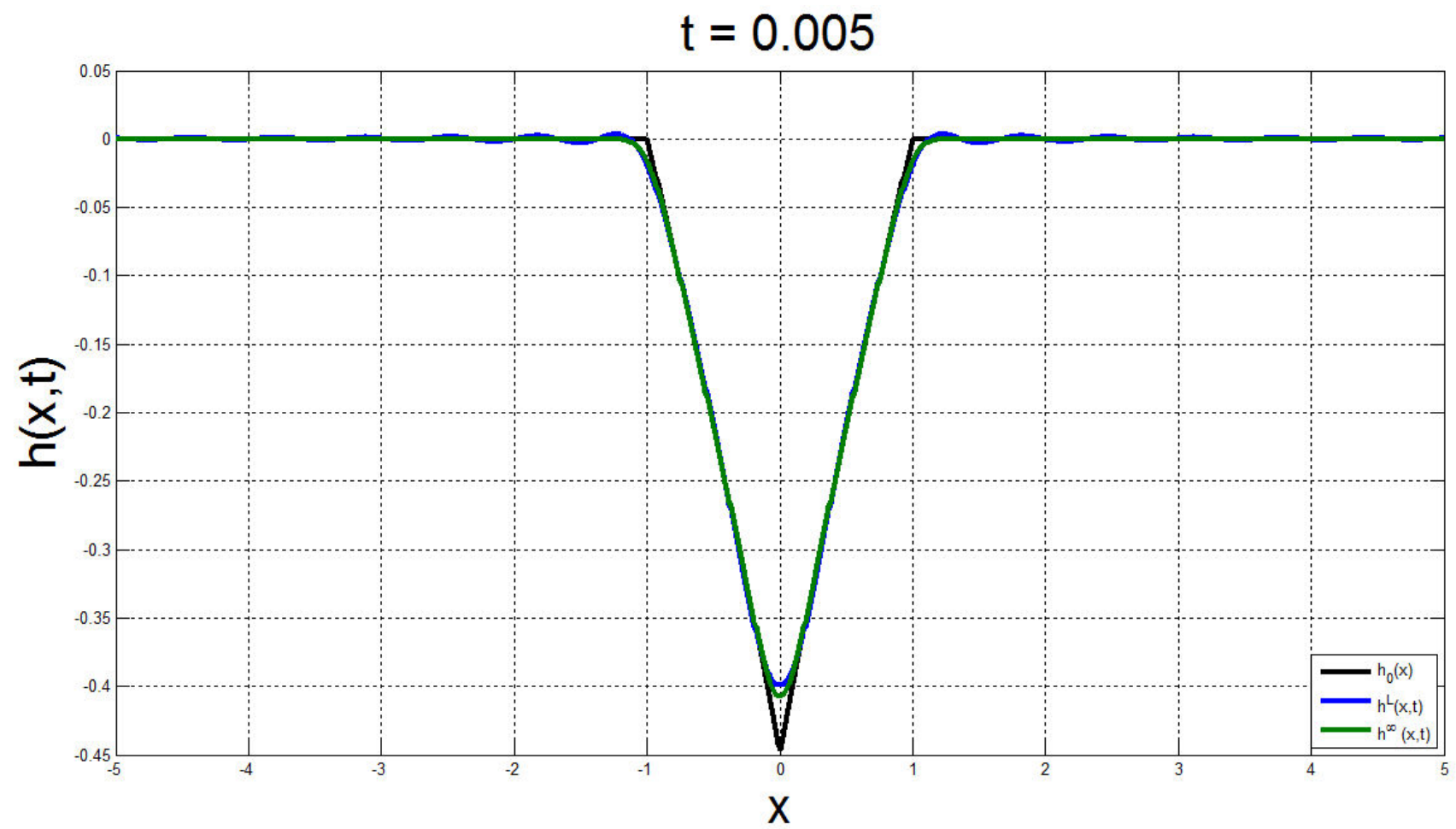
$t = 0.02$

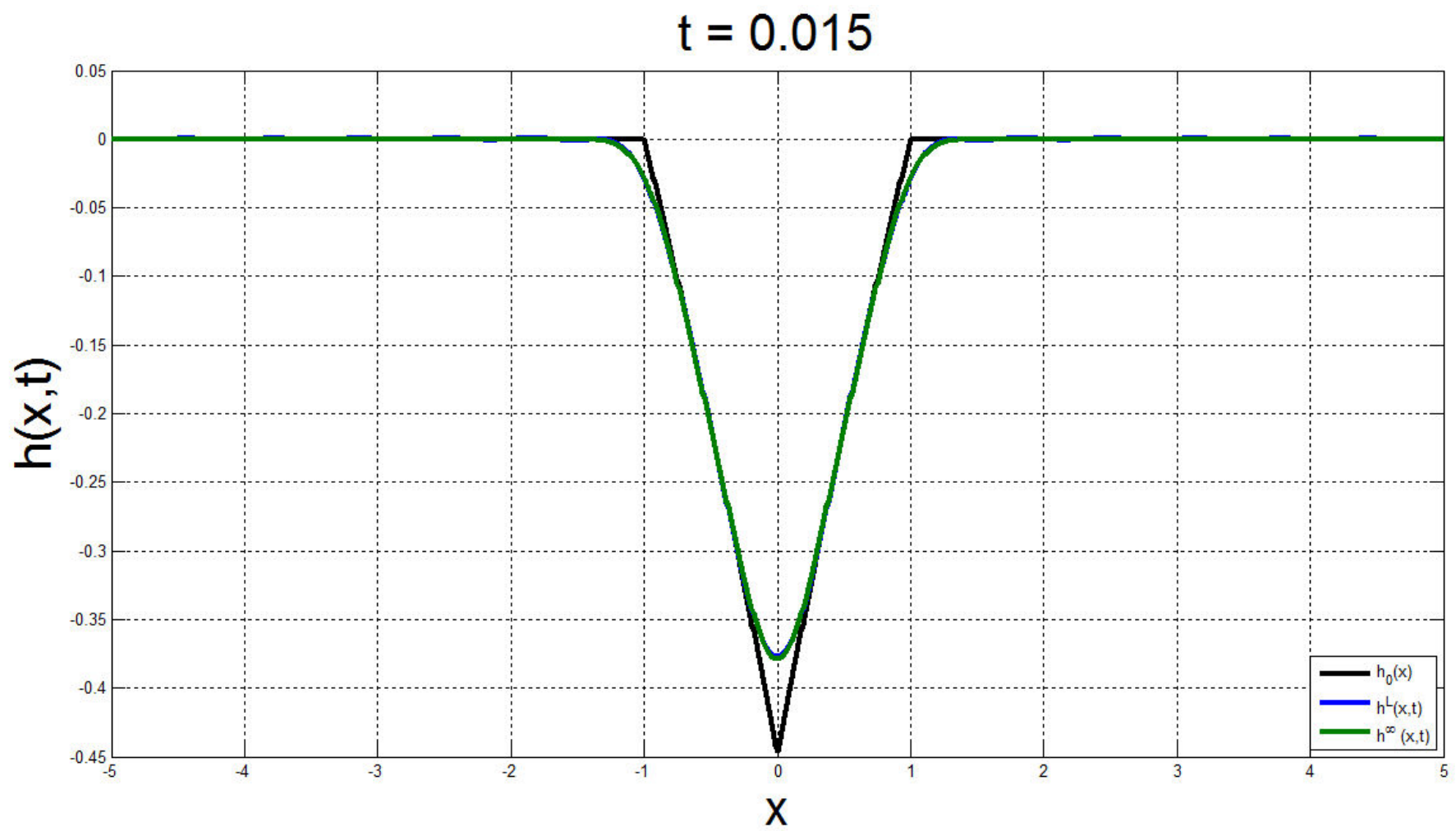


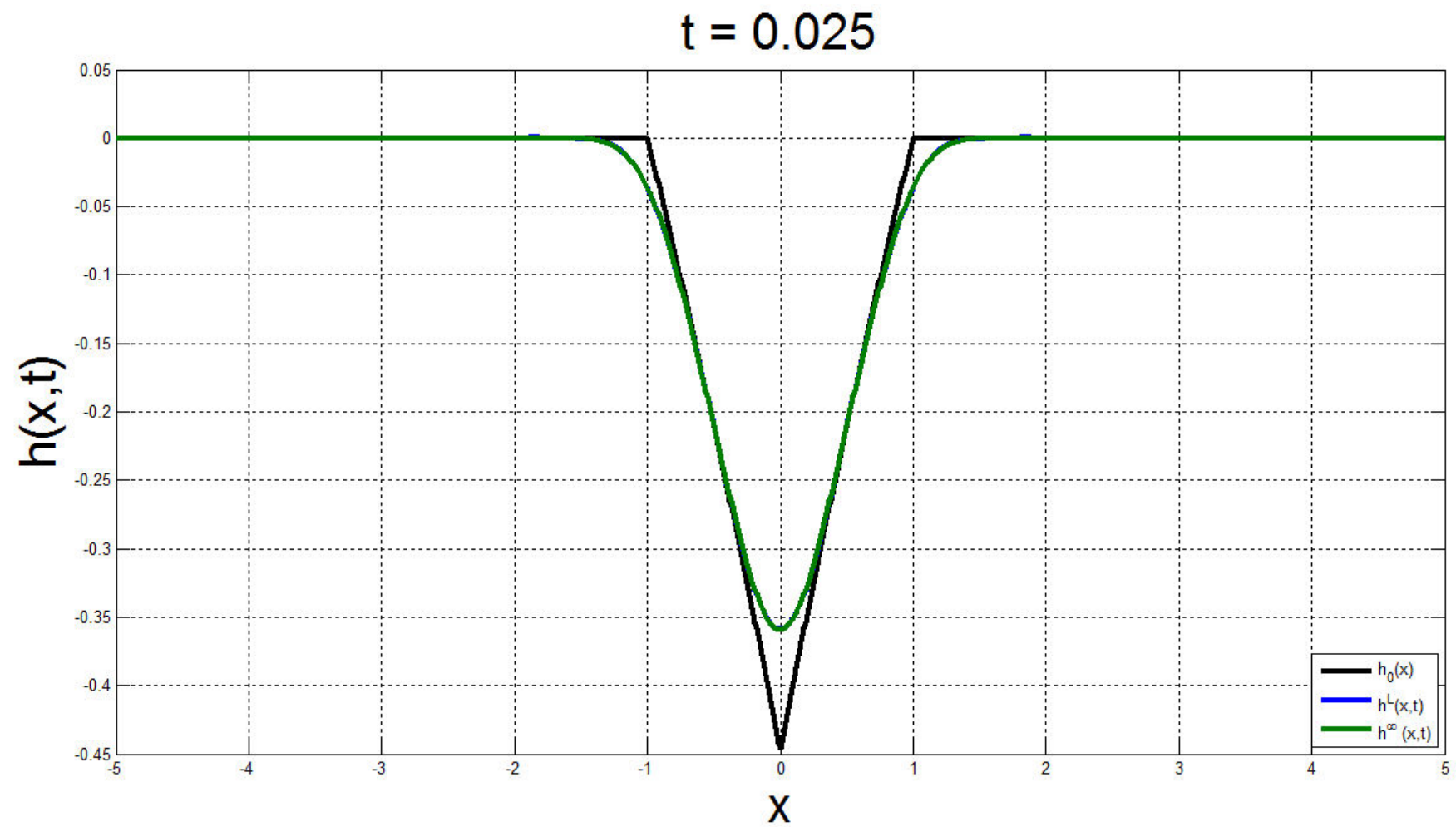
$t = 0.03$











Conclusion

**The KPZ equation forgets
about the presence of boundary
conditions quite quickly.**

**THANK YOU FOR
YOUR ATTENTION!**