From the Newton equation to the wave equation in some simple cases

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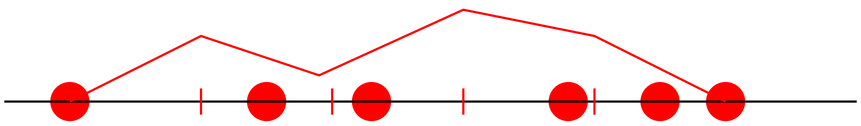
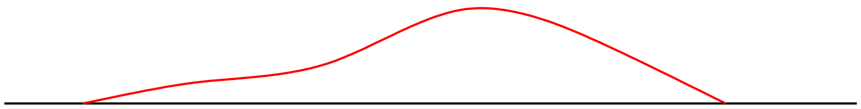
Outline

- Setting of the problem.
- Formal limit.
- Simple result: NN linear case.
- Simple result: NN nonlinear convex case.
- NNN linear case.
  - Natural assumptions: convexity issues
  - Convex case
  - Non convex case
- NNN nonlinear case: asymptotically linearized regime.

Setting of the problem





Newton equations :

$$\frac{d^2 X_i}{dt^2} = -\sum_{j \neq i} \nabla V(i - j + X_i - X_j)$$

Nonlinear wave equation :

$$\frac{\partial^2 \phi}{\partial \tau^2}(x, \tau) - \text{div } [D_A E(\nabla \phi)] = 0,$$

$$E(A) = \sum_{k \in \mathbf{Z}^d \setminus \{0\}} V(k + Ak), \text{ for } A \in \mathbb{R}^{d \times d}.$$

Link between these settings (in 1D) ?

Related works:

Berezhnyy/Berlyand 2006, E/Ming 2007, Ortner/Theil 2012.

Formal limit

$$\frac{d^2X_i}{dt^2} = -\sum_{j\neq i} \nabla V(i-j+X_i-X_j)$$

Assuming that $X_i(t) = N\phi\left(\frac{i}{N},\frac{t}{N}\right)$ and considering a macroscopic time $\tau = t/N$,

$$\frac{1}{N}\frac{\partial^2\phi}{\partial\tau^2}\left(\frac{i}{N},\frac{t}{N}\right) = -\sum_{j\neq i}\nabla V\left[i-j+N\left(\phi\left(\frac{i}{N},\frac{t}{N}\right)-\phi\left(\frac{j}{N},\frac{t}{N}\right)\right)\right].$$

As $N\to\infty$, we remark

$$N\left(\phi\left(\frac{i}{N},\frac{t}{N}\right)-\phi\left(\frac{j}{N},\frac{t}{N}\right)\right) \approx \nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)\cdot(i-j) - \frac{1}{2N}D^2\phi\left(\frac{i}{N},\frac{t}{N}\right)(i-j,i-j).$$

$$\frac{1}{N}\frac{\partial^2\phi}{\partial\tau^2}\left(\frac{i}{N},\frac{t}{N}\right) \approx \underbrace{\sum_{k\neq 0}\nabla V\left[k+\nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)\cdot k\right]}_{=0}$$

$$+\frac{1}{2N}\sum_{k\neq 0}\underbrace{D^2V\left[k+\nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)\cdot k\right]D^2\phi\left(\frac{i}{N},\frac{t}{N}\right)(k,k).}_{=\nabla\left[\nabla V\left(k+\nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)k\right)\cdot k\right]}$$

Formal limit

$$\frac{d^2 X_i}{dt^2} = -\sum_{j\neq i} \nabla V(i - j + X_i - X_j)$$

$$\frac{1}{N}\frac{\partial^2 \phi}{\partial \tau^2}\left(\frac{i}{N},\frac{t}{N}\right) \approx \frac{1}{2N}\sum_{k\neq 0}\nabla\left[\nabla V\left(k + \nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)k\right)\cdot k\right]$$

Assuming that $i/N \to x$, a fixed macroscopic point, we obtain

$$\frac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - \mathrm{div}\ \left[D_A E(\nabla\phi)\right] = 0,$$

where

$$E(A) = \sum_{k\in\mathbf{Z}^d\setminus\{0\}} V(k + Ak),$$

for $A \in \mathbb{R}^{d\times d}$.

Simplest case: NN linear

Nearest neighbour interaction:

$$\frac{d^2 X_i}{dt^2} = V'(1 + X_{i+1} - X_i) - V'(1 + X_i - X_{i-1})$$

with the convention that $X_0 = 0$, $X_{N+1} = 0$. Linear case: $V(x) = \frac{1}{2}(x-1)^2$.

$$\frac{d^2 X_i}{dt^2} = X_{i+1} - 2X_i + X_{i-1}.$$

Limit equation: $\phi\left(\frac{i}{N}, \frac{t}{N}\right) = \frac{1}{N} X_i(t)$.

$$\frac{\partial^2 \phi}{\partial \tau^2} = N^2 \left[\phi\left(\frac{i+1}{N}, \frac{t}{N}\right) - 2\phi\left(\frac{i}{N}, \frac{t}{N}\right) + \phi\left(\frac{i-1}{N}, \frac{t}{N}\right) \right].$$

$$\frac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - \frac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0.$$

Simplest case: NN linear

Proposition

Let $(\phi^0, \phi^1) \in \left[H^4(0,1)\right]^2$ be such that $\phi^0(0) = 0$ and $\phi^0(1) = 1$. Define, for all $N \in \mathbb{N}$, and for all $1 \leq i \leq N$,

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right).$$

Let $X_i(t)$ be the unique solution to the NN-linear Newton equation, with the convention $X_0 = 0,\ X_{N+1} = 0$, and let $\phi \in L^\infty\left(\mathbb{R}^+, H^1(0,1)\right)$ be the unique solution of linear-NN wave equation. Then, we have the convergences

$$\forall \tau > 0, \quad \sup_{1 \leq i \leq N} \left| \frac{1}{N} X_i(N\tau) - \phi\left(\frac{i}{N}, \tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and

$$\forall \tau > 0, \quad \left[\sup_{1 \leq i \leq N} \left| \frac{dX_i}{dt}(N\tau) - \frac{\partial \phi}{d\tau}\left(\frac{i}{N}, \tau\right)\right|\right] \underset{N\to\infty}{\longrightarrow} 0.$$

Proving the result amounts to proving convergence of a finite difference scheme.

Bottom line for Proof

For a function Φ, we denote by

$$D_\varepsilon \Phi(x) = \varepsilon^{-1}(\Phi(x+\varepsilon/2) - \Phi(x-\varepsilon/2)),$$

where, of course, ε plays the role of $1/N$. This discrete differentiation can be iterated:

$$D_\varepsilon^2 \Phi = \varepsilon^{-2}(\Phi(x+\varepsilon) - 2\Phi(x) + \Phi(x-\varepsilon)).$$

Using this notation, proving (after renormalization in time) the convergence of the solution to the Newton equation to the solution to the wave equation basically amounts to proving (if we omit the truncation error terms) that the solution Φ_ε to

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - D_\varepsilon^2 \Phi_\varepsilon = 0,$$

with suitable (vanishing) initial and boundary conditions, vanishes with ε. This is an immediate consequence of the fact that Φ_ε satisfies the energy equality

$$\frac{d}{dt}\left(\left\| \frac{\partial}{\partial t}\Phi_\varepsilon \right\|^2 + \|D_\varepsilon \Phi_\varepsilon\|^2 \right) = 0.$$

Simple case: NN nonlinear convex

Nearest neighbour interaction:

$$\frac{d^2 X_i}{dt^2} = V'(1 + X_{i+1} - X_i) - V'(1 + X_i - X_{i-1})$$

with the convention that $X_0 = 0$, $X_{N+1} = 0$.

Limit equation: $\phi\left(\frac{i}{N}, \frac{t}{N}\right) = \frac{1}{N} X_i(t)$.

$$\frac{\partial^2 \phi}{\partial \tau^2} = N\Bigg[V'\left[1 + N\left(\phi\left(\frac{i+1}{N}, \frac{t}{N}\right) - \phi\left(\frac{i}{N}, \frac{t}{N}\right)\right)\right] \\ - V'\left[1 + N\left(\phi\left(\frac{i}{N}, \frac{t}{N}\right) - \phi\left(\frac{i-1}{N}, \frac{t}{N}\right)\right)\right]\Bigg].$$

$$\frac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - \frac{\partial}{\partial x}\left[V'\left(1 + \frac{\partial \phi}{\partial x}\right)\right] = 0.$$

Simple case: NN nonlinear convex

Proposition

Assume that $V \in C^4$, $V'(1) = 0$ and that $V'' \geq \alpha > 0$ for some constant α. Assume that $\phi \in C^0\left([0,T), C^4([0,1])\right)$. Let $N \in \mathbb{N}$, and define, for all $1 \leq i \leq N$,

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right).$$

Let $X_i(t)$ be the unique solution to the NN nonlinear equation, with the convention $X_0 = 0,\ X_{N+1} = 0$. Then, we have the convergences

$$\forall \tau \in (0,T), \qquad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and

$$\forall \tau \in (0,T), \qquad \sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0.$$

Proof: similar to the linear case.

NNN linear non convex

$$\frac{d^2 X_i}{dt^2} = c_1 (X_{i+1} - 2X_i + X_{i-1}) + c_2 (X_{i+2} - 2X_i + X_{i-2})$$

The (formal) limit reads:

$$\frac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - (c_1 + 4c_2)\,\frac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0,$$

which is well-posed iff $c_1 + 4c_2 > 0$.

Special case: $c_1 > 0, c_2 > 0$. Then the NN proof applies:

$$\frac{d}{dt}\left(\left\| \frac{\partial}{\partial t}\Phi_\varepsilon \right\|^2 + c_1 \left\| D_\varepsilon \Phi_\varepsilon \right\|^2 + 4\, c_2 \left\| D_{2\varepsilon} \Phi_\varepsilon \right\|^2 \right) = 0.$$

What about the case when $c_1 + 4c_2 > 0$ only?

NNN linear nonconvex

$$\frac{d^2 X_i}{dt^2} = c_1(X_{i+1} - 2X_i + X_{i-1}) + c_2(X_{i+2} - 2X_i + X_{i-2})$$

This also reads $\frac{d^2 X}{dt^2} = -c_1 AX - c_2 BX$, with

$$A = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}, \quad \text{and} \quad B = \begin{pmatrix} 2 & 0 & -1 & 0 & \cdots & 0 \\ 0 & 2 & 0 & -1 & \ddots & \vdots \\ -1 & 0 & 2 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & -1 \\ \vdots & \ddots & -1 & 0 & 2 & 0 \\ 0 & \cdots & 0 & -1 & 0 & 2 \end{pmatrix}.$$

First miracle: $B = 4A - A^2$.

NNN linear nonconvex

$$\frac{d^2X}{dt^2} = -c_1AX - c_2BX = -(c_1+4c_2)AX + c_2A^2X,$$

Second miracle: the spectrum of A is explicit

$$\lambda_k = 4\sin^2\left(\frac{k\pi}{2(N+2)}\right),$$

$$(u_k)_i = \sin\left(\frac{ik\pi}{N+2}\right),$$

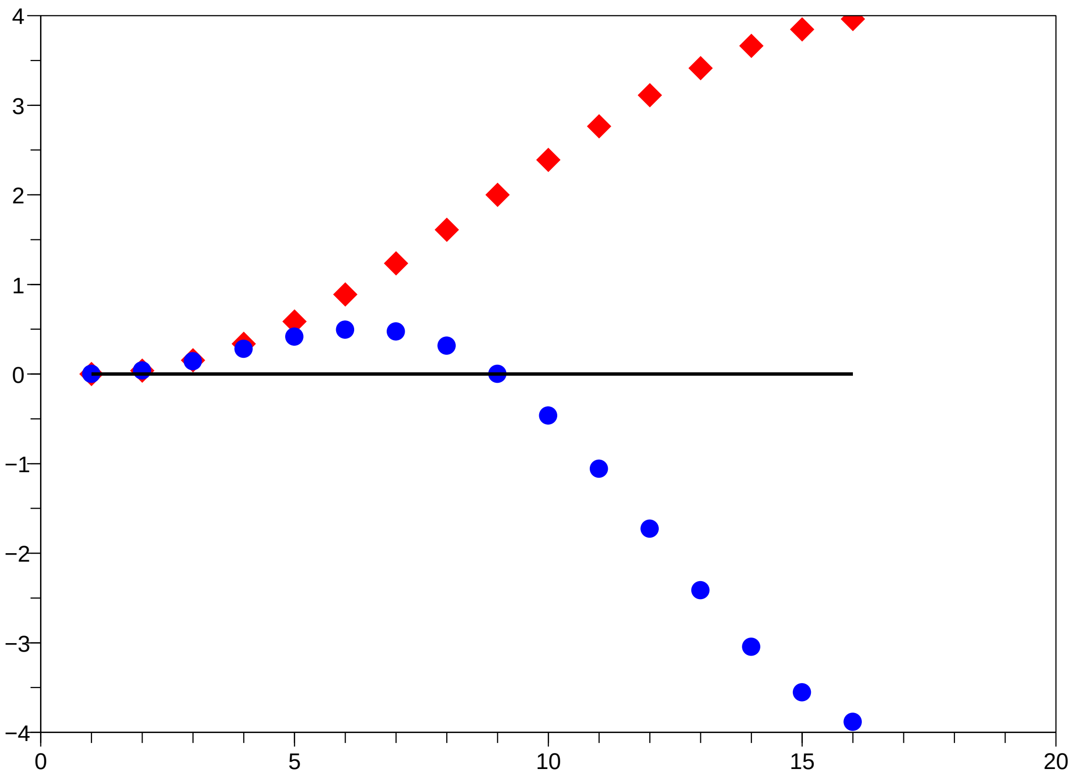
If $c_1 < 0$,

$$\mu_k := (c_1+4c_2)\lambda_k - c_2\lambda_k^2 < 0$$

is possible: exponential growth in time

$$\frac{d^2x}{dt^2} = -\mu_k x \quad \Rightarrow \quad x(t) = x(0)\cosh(\sqrt{-\mu_k}t) + \frac{dx}{dt}(0)\frac{1}{\sqrt{-\mu_k}}\sinh(\sqrt{-\mu_k}t).$$

NNN linear nonconvex



Eigenvalues λ_k (♦) and $\mu_k = (c_1 + 4c_2)\lambda_k - c_2\lambda_k^2$ (●) with $c_1 = -1, c_2 = 0.5$

NNN linear nonconvex

Proposition

Assume that $c_1 + 4c_2 > 0$, and that ϕ is the solution to the wave equation, with $\phi^0, \phi^1 \in C^4(0,1)$. Assume that the functions ϕ^0 and ϕ^1 satisfy

$$\exists C > 0, \quad \exists \theta > 0, \quad \text{s.t.} \quad \forall k \in \mathbb{N}^*, \quad \left|\widehat{\phi^0}(k)\right| + \left|\widehat{\phi^1}(k)\right| \leq C e^{-\theta k}.$$

For any $N \in \mathbb{N}$, define

$$\forall 0 \leq i \leq N, \quad X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right),$$

and let X_i be the unique solution to the Newton equations. Then, we have the convergences

$$\forall \tau > 0, \quad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and

$$\forall \tau > 0, \quad \sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0.$$

NNN linear nonconvex

A proof by weak convergence

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - (c_1 + 4c_2) D_\varepsilon^2 \Phi_\varepsilon + c_2 \varepsilon^2 D_\varepsilon^4 \Phi_\varepsilon = 0.$$

Energy estimate:

$$\frac{d}{dt} \left(\left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \left\| D_\varepsilon \Phi_\varepsilon \right\|^2 - c_2 \varepsilon^2 \left\| D_\varepsilon^2 \Phi_\varepsilon \right\|^2 \right) = 0.$$

Differentiate k times the equation and obtain a similar energy estimate

$$\frac{d}{dt} \left(\left\| D_\varepsilon^k \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \left\| D_\varepsilon^{k+1} \Phi_\varepsilon \right\|^2 - c_2 \varepsilon^2 \left\| D_\varepsilon^{k+2} \Phi_\varepsilon \right\|^2 \right) = 0.$$

for each differentiation order k. In order to “eliminate” the nonpositive contribution of the last term, we now weight and combine all these estimates so as to obtain

$$\frac{d}{dt} \sum_{k=1}^{+\infty} \delta^{2k} \left(\left\| D_\varepsilon^k \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \left\| D_\varepsilon^{k+1} \Phi_\varepsilon \right\|^2 - c_2 \varepsilon^2 \left\| D_\varepsilon^{k+2} \Phi_\varepsilon \right\|^2 \right) = 0.$$

NNN linear nonconvex

This parameter δ is next adjusted, in function of ε, so as to cancel the series of the two right-most terms by making it a telescopic series. We therefore conclude that some norm of the form

$$\sum_{k=1}^{+\infty} \delta^{2k} \left\| D_\varepsilon^{k+1} \Phi_\varepsilon \right\|^2$$

remains bounded over time.

Up to an extraction, we may assume Φ_ε is weakly convergent, and it remains to deduce that the convergence is strong.

This will be a consequence of the preservation of the energy by the equation, and the fact that strong convergence holds at initial time.

NNN linear nonconvex

Proposition

Assume that $c_1 + 4c_2 > 0$, and that ϕ is the solution to the wave equation, with initial data $\phi^0, \phi^1 \in H^1(0,1)$. Consider the initial conditions $N\phi^0\left(\frac{i}{N}\right)$ and $\phi^1\left(\frac{i}{N}\right)$ for Newton equations. There exists a filtered initial condition X_i^0, V_i^0 such that

$$\sup_{1\leq i\leq N}\left|\frac{1}{N}X_i^0 - \phi^0\left(\frac{i}{N}\right)\right| + \left|V_i^0 - \phi^1\left(\frac{i}{N}\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and, denoting by X_i the unique solution to the Newton equations with initial condition X_i^0, V_i^0,

$$\forall \tau > 0, \quad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and

$$\forall \tau > 0, \quad \sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0.$$

NNN nonlinear cases: linearized regimes

We introduce a parameter $\gamma \in (0,1)$ and modify the (say NN) Newton equation as follows:

$$\frac{d^2 X_i}{dt^2} = N^\gamma \left[V_1' \left(1 + \frac{X_{i+1} - X_i}{N^\gamma} \right) - V_1' \left(1 + \frac{X_i - X_{i-1}}{N^\gamma} \right) \right. \\ \left. + V_2' \left(2 + \frac{X_{i+2} - X_i}{N^\gamma} \right) - V_2' \left(2 + \frac{X_i - X_{i-2}}{N^\gamma} \right) \right],$$

Then we can prove that the corresponding limit is

$$\frac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - \left(V_1''(1) + 4V_2''(2) \right) \frac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0,$$

Remark: We have no clue on the nonlinear nonconvex non-linearized case.

NNN nonlinear nonconvex but linearized

Formal idea:

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - \varepsilon^{\gamma-1} D_\varepsilon \nabla V(\varepsilon^{1-\gamma} D_\varepsilon \Phi_\varepsilon) = 0,$$

When $\gamma \in (0,1)$, we observe that, still formally, Φ_ε converges to the solution Φ to

$$\frac{\partial^2 \Phi}{\partial t^2} - \nabla V(0).D^2\Phi = 0.$$

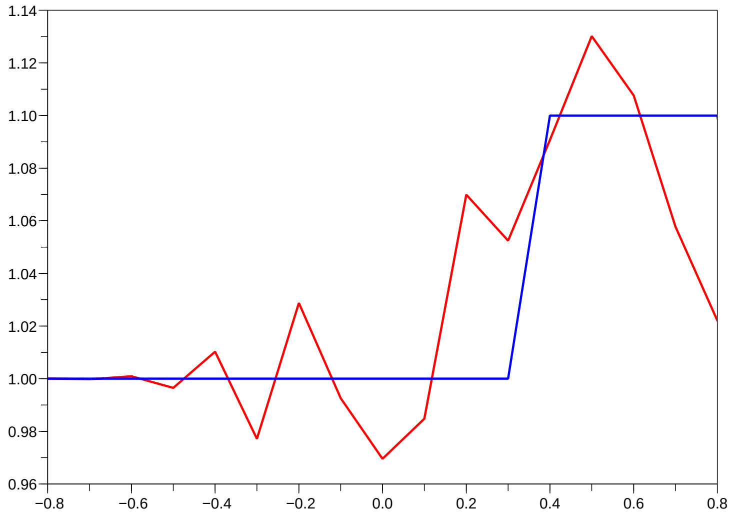
Proof using our "weak convergence + energy conservation" technique.

It is beyond our reach, without assuming convexity and thus simply using weak convergence arguments, to determine the limit of a term like $D_\varepsilon \nabla V(D_\varepsilon \Phi_\varepsilon)$ unless ∇V is linear. This explains why, in the present state of our understanding, we need to resort to the specific normalization using $\gamma \in (0,1)$.

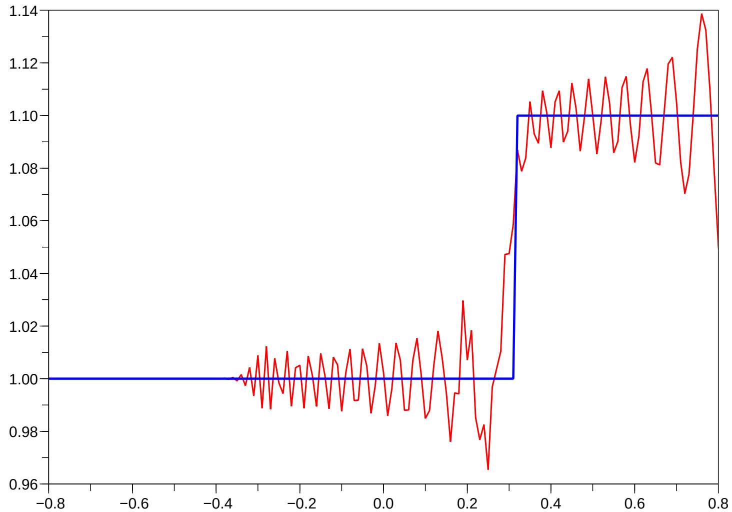
Shocks

The nonlinear wave equation may develop shocks.

The "numerical scheme" defined by Newton equation does not dissipate (numerical) entropy.

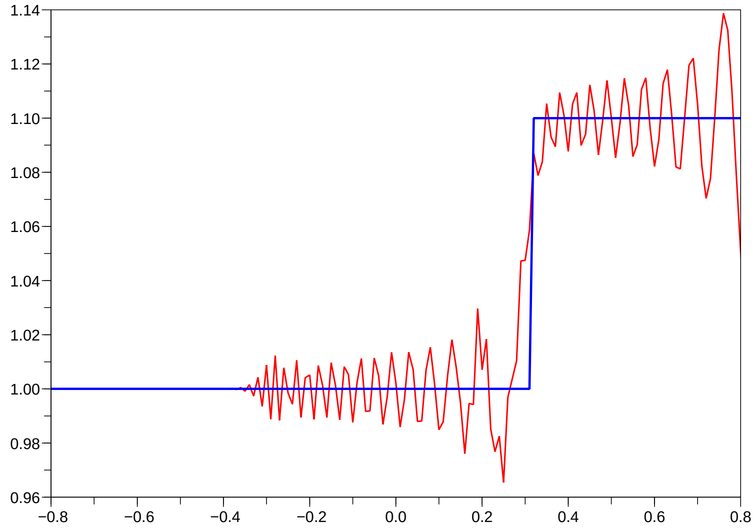


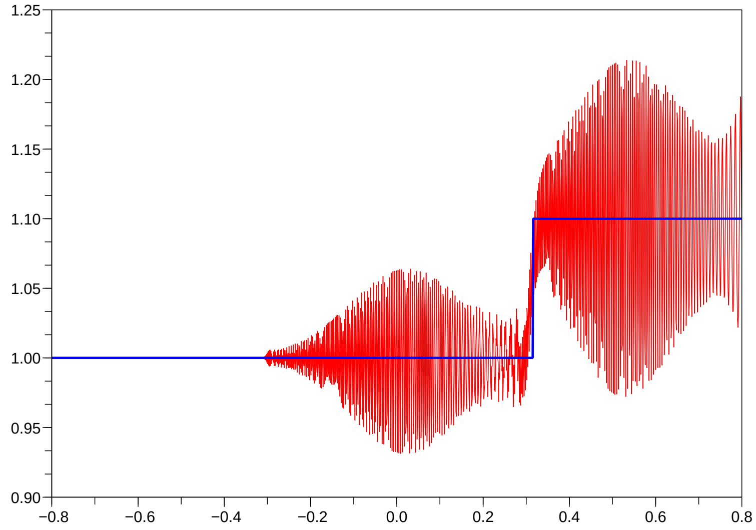
$N = 10$



$N = 100$

Shocks





$N = 100$ $N = 1000$

Shocks

Test of weak convergence: