A Simplified One-Dimensional Model of Shock and Detonation Waves

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http://cermics.enpc.fr/∼stoltz/

References

- G. Stoltz, *Shock waves in an augmented one-dimensional atom chain*, Nonlinearity **18** (2005) 1967-1985
- Presentation and preprints available at the URL `http://cermics.enpc.fr/~stoltz/`

Why looking for a simplified model?

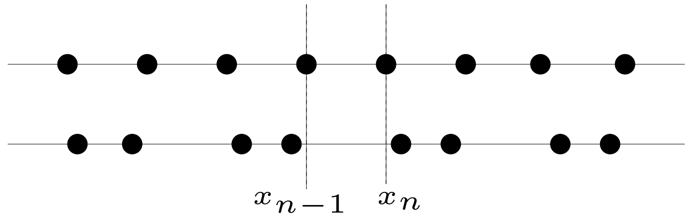
- Shock/detonation waves are multiscale phenomena
- Different descriptions (fluid dynamics, molecular dynamics)
- Usually, MD is used to calibrate parameters
- A direct micro/macro limit (at least in some asymptotic regime) would be very interesting
- Hence simplified 1D model since mathematical results on 1D chains exist?

Outline of the talk

- Shock waves in one dimensional chains
- Introducing some mean higher dimensional perturbations
  - some heuristical forcing term
  - a bath of linear oscillators and its stochastic limit
  - a nonlinear model
- Extension to detonation waves
  - a simplified model of detonation in 1D chains
  - some numerical results

I. Shock waves in one-dimensional atom chains

The model



- Consider the Hamiltonian (nearest-neighbor interactions):

$$H_{\mathsf{s}}(\{q_n,\, p_n\}) = \sum_{n=-\infty}^{\infty} V(q_{n+1} - q_n) + \frac{1}{2}\dot{p}_n^2, \tag{1}$$

  with $(q_n, p_n) = (x_n, \dot{x}_n)$ (x_n = displacement, not position!).

- Newton's equations of motion:

$$\ddot{x}_n = V'(x_{n+1} - x_n) - V'(x_n - x_{n-1}). \tag{2}$$

- Usually, Lennard-Jones like potential (possibly Morse or Toda)
- Normalization conditions $V(0) = 0, \;\; V'(0) = 0, \;\; V''(0) = 1$
- $b = -V'''(0)$ measures at the first order the anharmonicity of the system

Shocks in the 1D chain

- Shock obtained by compression by an infinitely massive piston (velocity u_p)[a]
- Classification of the shock regimes according to $a = b\, u_p$:
  - $a < 2$ = harmonic like behavior
  - $a > 2$ = hard rod like behavior
- Rigorous mathematical proof in the Toda case[b]
- Robustness of the profiles with respect to thermal inital conditions / averaging over several realizations

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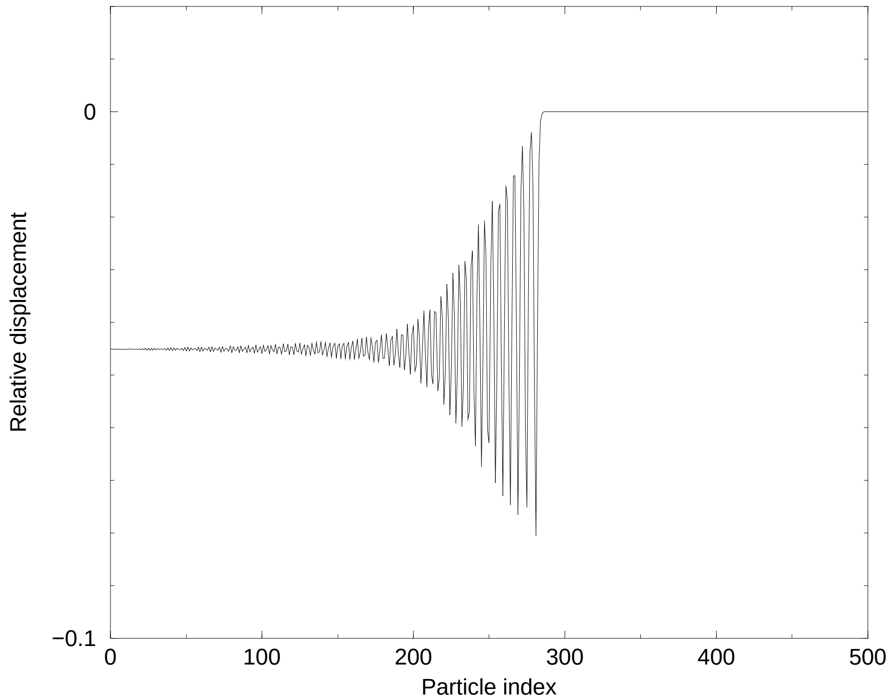
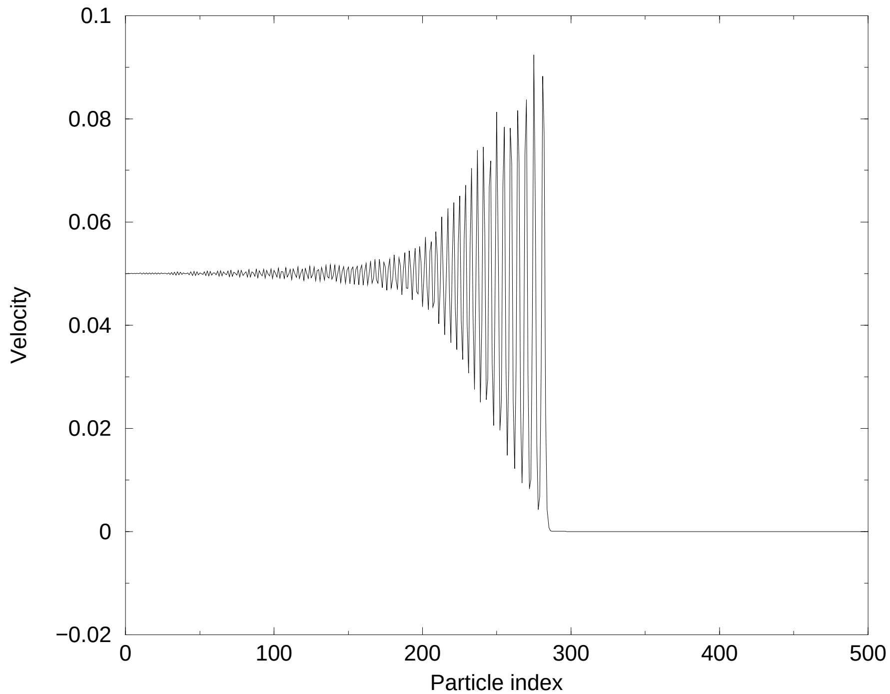
[a] Duvall *et al.* (1969); Holian *et al.* (1978, 1979, 1981)
[b] Venakides *et al.* (1991)

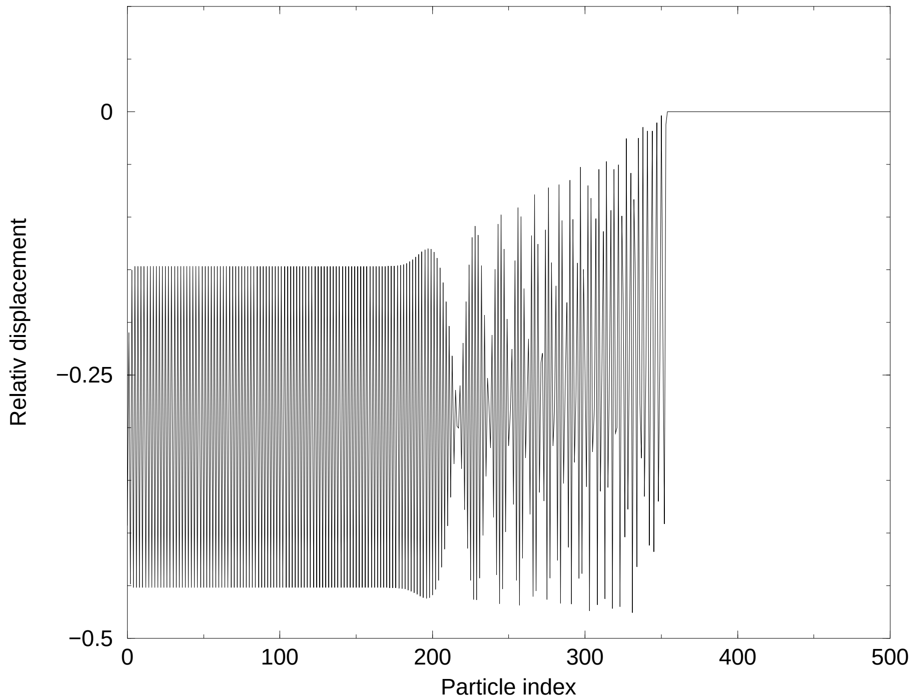
Weak shock profiles ($a < 2$)

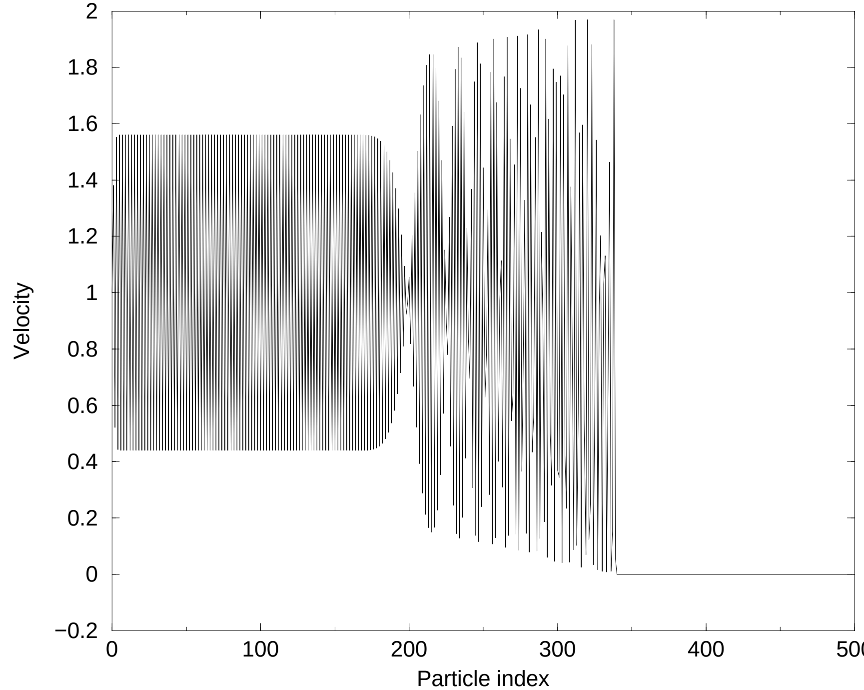




Weak shock profiles ($a = 0.45$) for a Lennard-Jones like potential for particles initially at rest. Left: Relative displacement profile ($x_{n+1} - x_n$). Right: Particle velocity. The sizes of the different regions grow linearly in time.

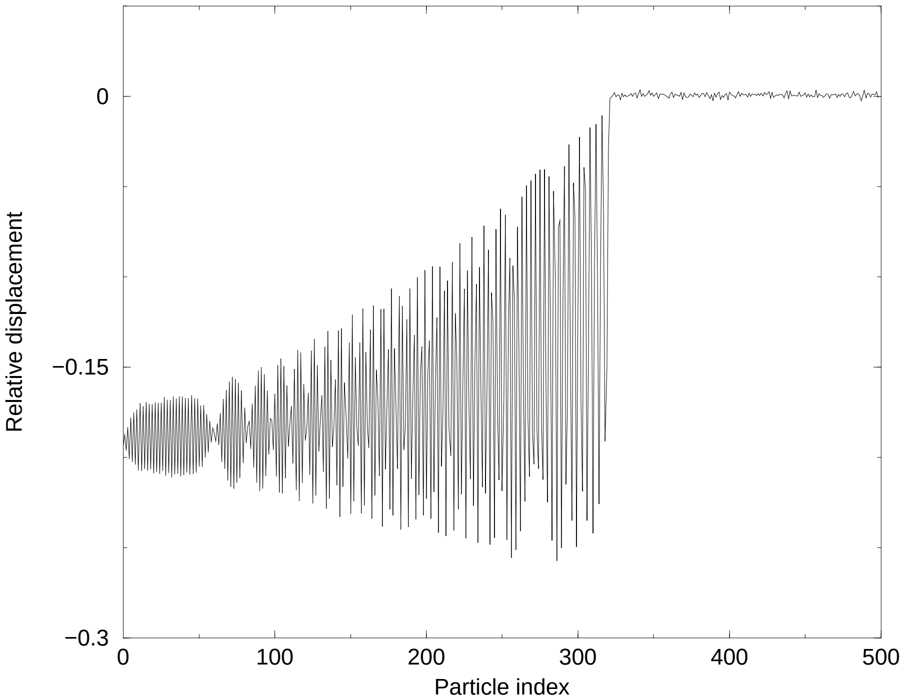
Strong shock profiles ($a > 2$)

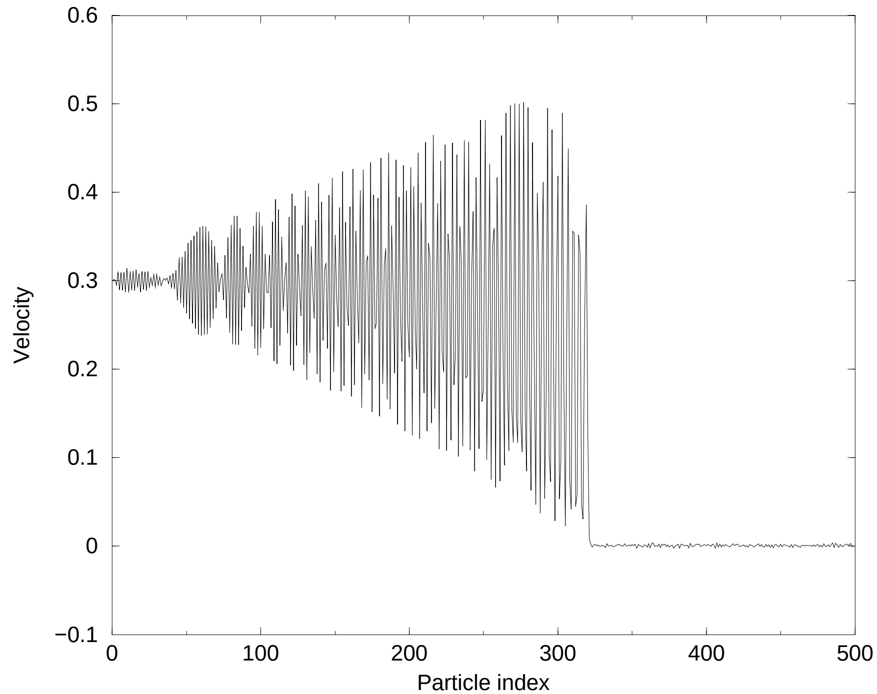




Strong shock profiles ($a = 9$) for a Lennard-Jones like potential for particles initially at rest. Left: Relative displacement profile ($x_{n+1} - x_n$). Right: Particle velocity. The sizes of the different regions grow linearly in time. Relaxation waves are problematic (soliton train not damped out).

Thermalized strong shock profiles ($a > 2$)





Strong shock profiles ($a = 9$) for a Lennard-Jones like potential for particles initially at rest. Left: Relative displacement profile ($x_{n+1} - x_n$). Right: Particle velocity. The initial temperature is $\beta^{-1} = 0.01$.

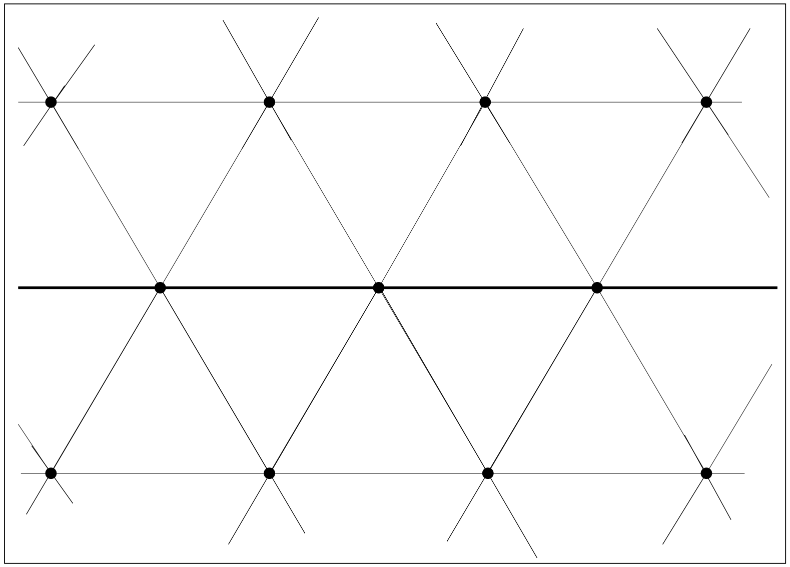
II. Introducing some mean higher dimensional perturbations

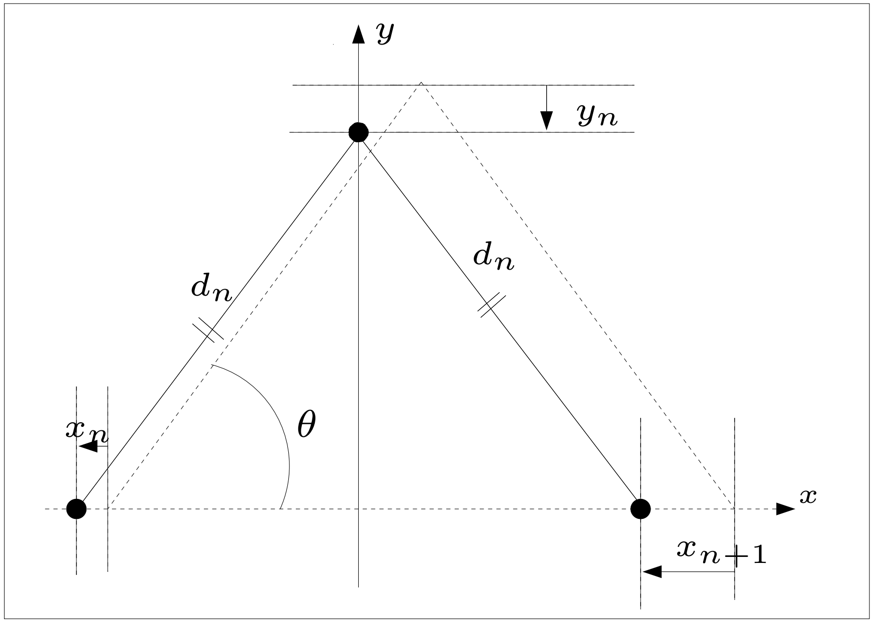
3D is not 1D

- 1D shocks behave badly because there is no room for relaxation (formation of the most energetic waves = binary waves)
- 3D shocks are 1D like only at $T = 0$ and when the compression is done along a principal axis[a]
- Otherwise, local equilibrium is quickly restored after the shock front has passed
- Idea: the transverse degrees of freedom are necessary for this relaxation = thermostat like degrees of freedom!

[a] Holian, *Shock waves* (1995)

The form of the transverse perturbations





Assumption: constrained d.o.f in the tranverse and longitudinal directions

For harmonic potentials (FCC <100> structure):

$$\ddot{x}_n = \frac{9}{8}(x_{n+1} - 2x_n + x_{n-1}) + \frac{\sqrt{3}}{4}(y_n - y_{n-1}), \quad \ddot{y}_n = -\frac{3}{2}y_n - \frac{\sqrt{3}}{2}(x_{n+1} - x_n)$$

General case: sum of potentials with different spring constants

The augmented 1D model

- System (S) and a heat bath (B) described by bath variables $\{y_n^j\}$ ($n \in \mathbb{Z},\ j = 1, \ldots, N$).
- The full Hamiltonian reads:

$$H(\{q_n,\, p_n,\, \tilde{q}_n^j,\, \tilde{p}_n^j\}) = H_{\mathsf{S}}(\{q_n,\, p_n\}) + H_{\mathsf{SB}}(\{q_n,\, p_n,\, \tilde{q}_n^j,\, \tilde{p}_n^j\}), \tag{3}$$

where $(q_n, p_n,\ \tilde{q}_n^j, \tilde{p}_n^j) = (x_n, \dot{x}_n, y_n^j, m_j \dot{y}_n^j)$, H_{S} is given by (1), and

$$H_{\mathsf{SB}} = \sum_{n=-\infty}^{\infty} \sum_{j=1}^{N} \frac{1}{2m_j} (\tilde{p}_n^j)^2 + \frac{1}{2} k_j \left[\gamma_j (x_{n+1} - x_n) + y_n^j\right]^2 . \tag{4}$$

- Interpretation: each longitudinal spring length is thermostated
- Spectrum $\omega_j^2 = k_j$, coupling constants γ_j

Choice of the spectrum parameters

- Compute the solutions for y, and insert it into the equations for x:

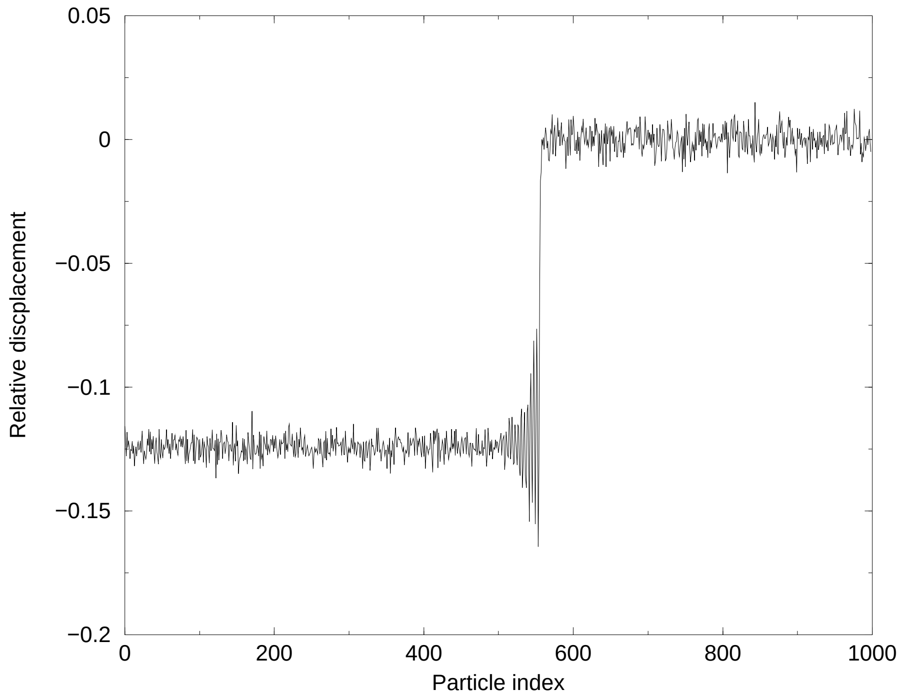
$$\begin{aligned}\ddot{x}_n(t) = \quad & V'(x_{n+1} - x_n) - V'(x_n - x_{n-1}) \\ & + \int_0^t K_N(t-s)(\dot{x}_{n+1} - 2\dot{x}_n + \dot{x}_{n-1})(s)\, ds + \sigma_n^N(t)\end{aligned}$$

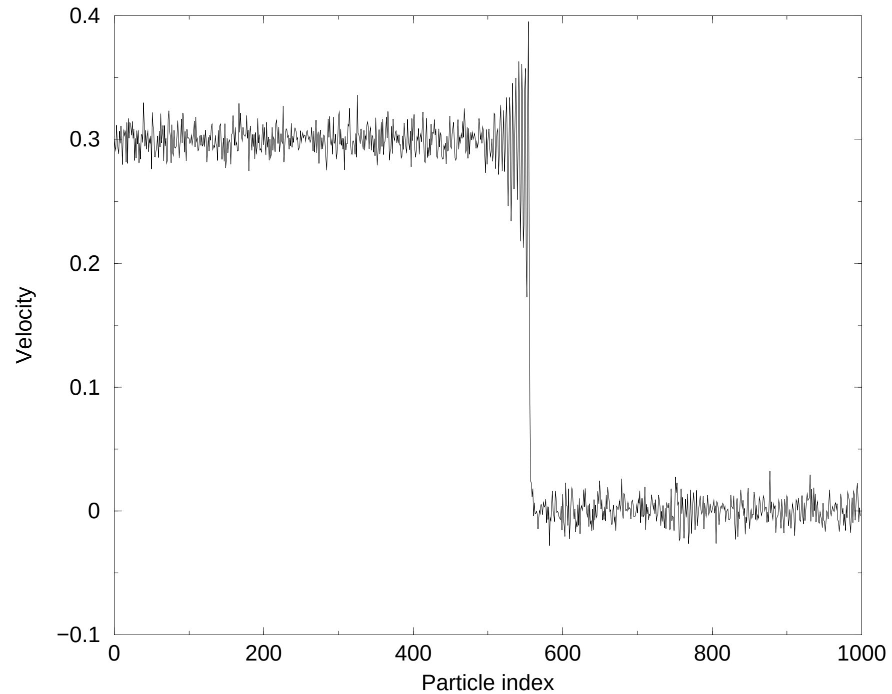
- σ random forcing term
- memory kernel $K_N(t) = \sum_{j=1}^N \gamma_j^2 \omega_j^2 \cos(\omega_j t)$ ("generalized Langevin equation")
- Exponentially decreasing in time ($\mathrm{e}^{-\alpha t}$) in the limit $N \to +\infty$ for the choice

$$\omega_j = \Omega \left(\frac{j}{N} \right)^k, \quad \gamma_j^2 \omega_j^2 = \lambda^2 f^2(\omega_j)\, (\Delta\omega)_j,$$

with $f^2(\omega) = \frac{2\alpha}{\pi} \frac{1}{\alpha^2+\omega^2}$, $(\Delta\omega)_j = \omega_{j+1} - \omega_j$, $\alpha, \lambda > 0$ and $k > 0$

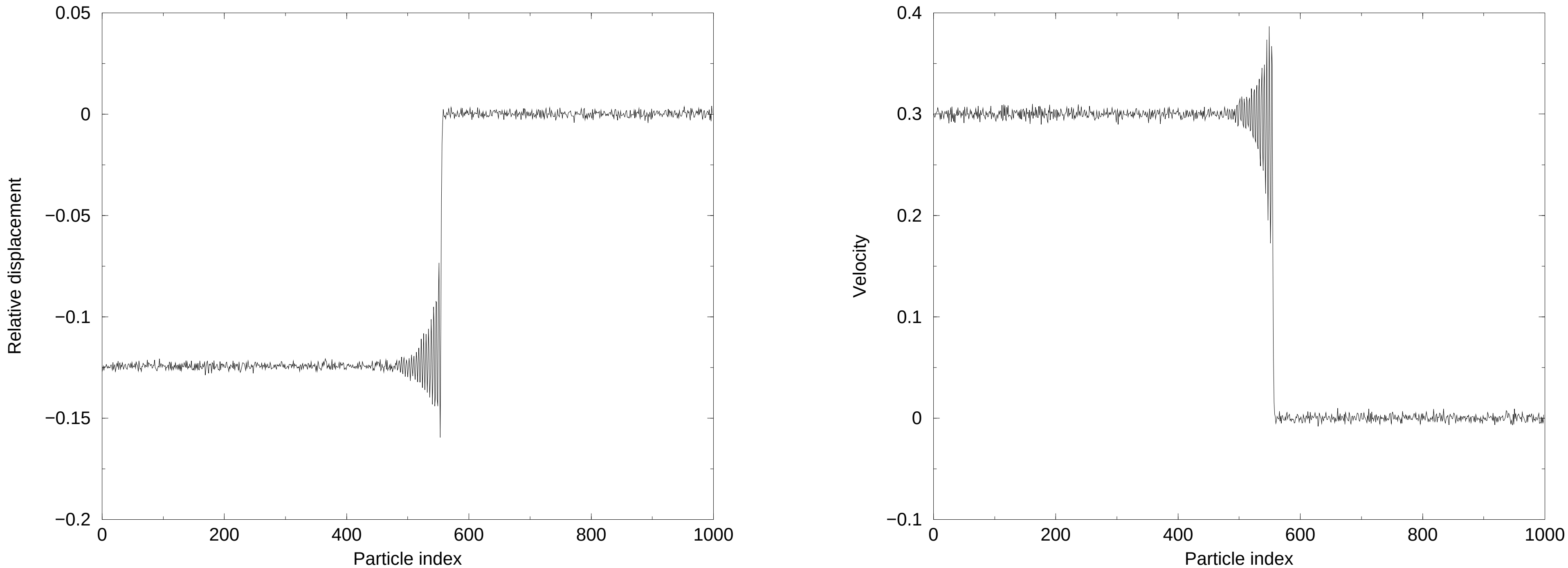
Some numerical results





Strong shock ($a = 3$) with $N = 200$, $k = 1$, $\Omega = 5$, $\alpha = 2$ and $\lambda = 1$. Left: Relative displacement profile. Right: Velocity profile.

Some numerical results (2)



Same parameters, but results averaged over 10 realizations. Notice that there remain oscillations at the shock front (similar results exist for 3D shocks[a])

[a] Zybin *et al.* (1999)

A nonlinear bath model

- Thermostating with less tranverse variables and for stronger shocks
- Model

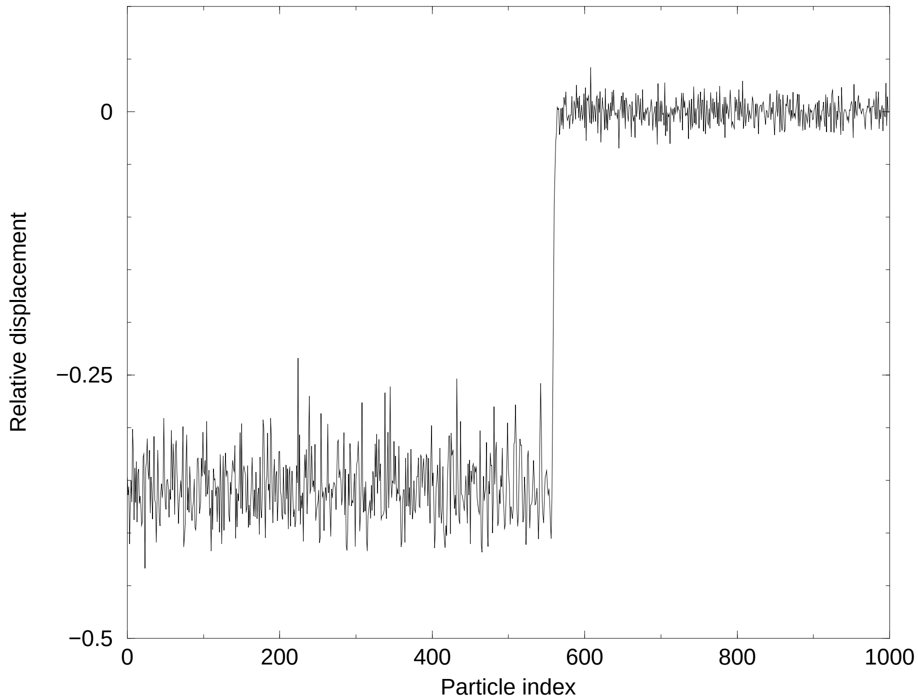
$$H(\{q_n,\, p_n,\, \tilde{q}_n^j,\, \tilde{p}_n^j\}) = H_{\mathsf{S}}(\{q_n,\, p_n\}) + H_{\mathsf{NLB}}(\{q_n,\, p_n,\, \tilde{q}_n^j,\, \tilde{p}_n^j\}), \qquad (5)$$

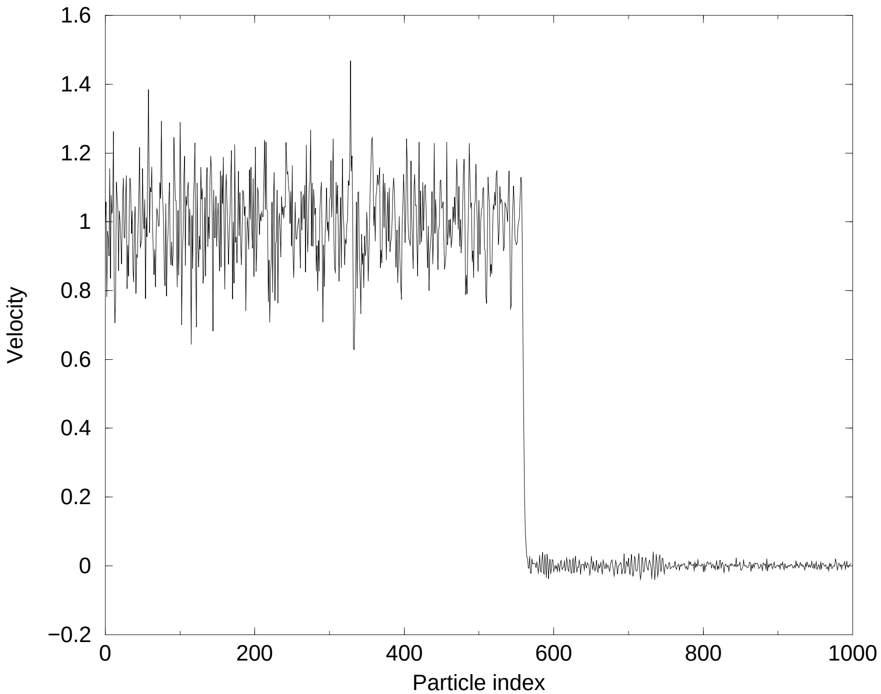
with

$$H_{\mathsf{NLB}} = \sum_{n=-\infty}^{\infty} \sum_{j=1}^{N} \frac{1}{2}(\tilde{p}_n^j)^2 + k_j U[\gamma_j(q_{n+1} - q_n) + \tilde{q}_n^j], \qquad (6)$$

- Typically, Lennard-Jones like interaction $U(x) = V_{\mathrm{LJ}}(1 + x)$

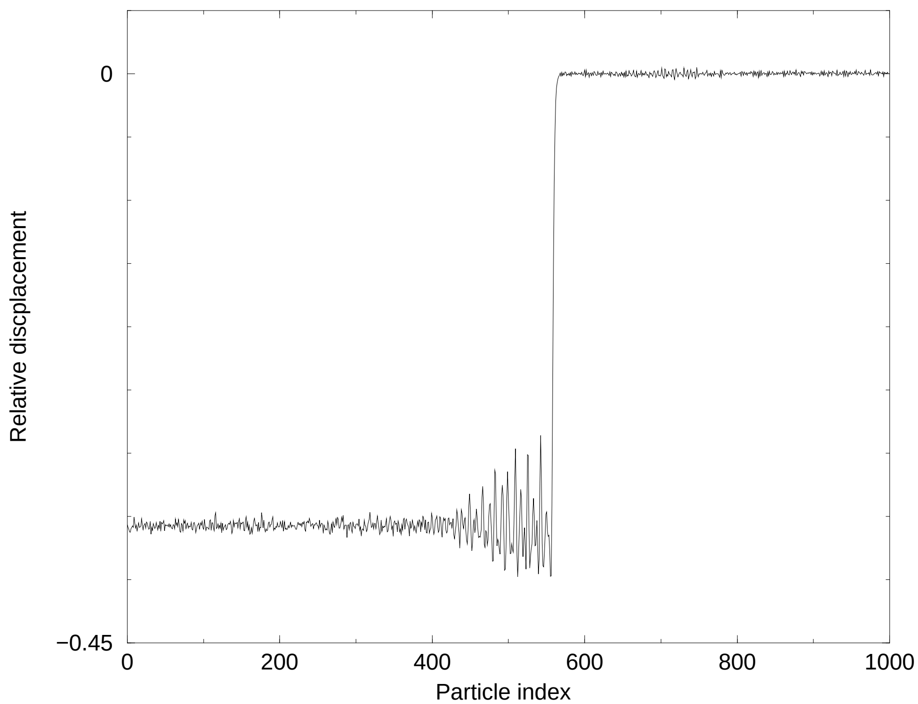
Some numerical results

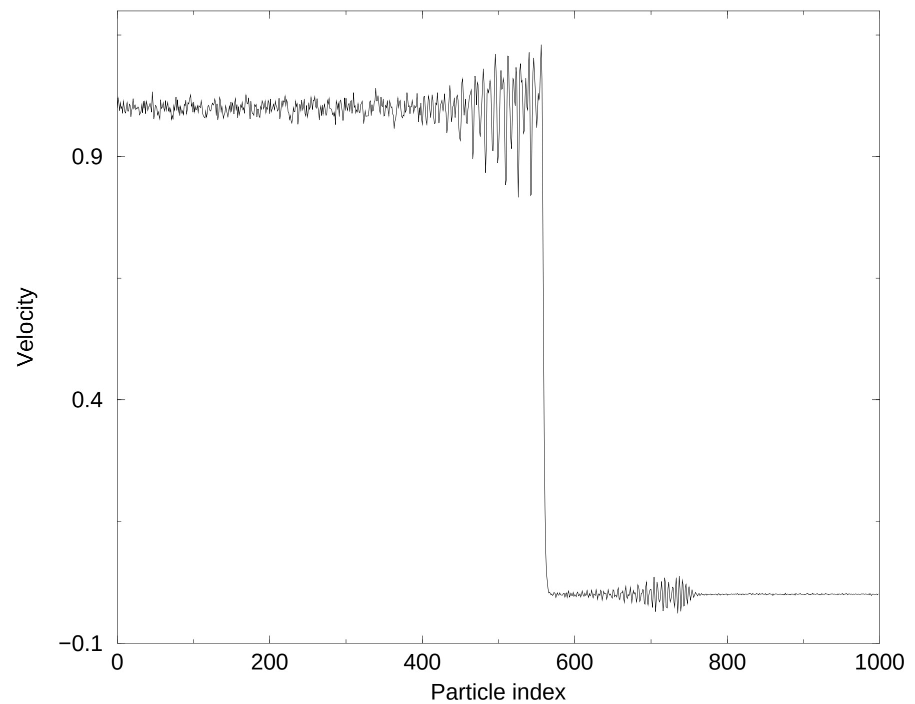




Strong shock ($u_p = 1$) with $N = 8$ NL oscillators, $k = 1$, $\Omega = 10$, $\alpha = 5$ and $\lambda = 0.2$. Left: Relative displacement profile. Right: Velocity profile.

Some numerical results (2)





Same parameters, but results averaged over 100 realizations.

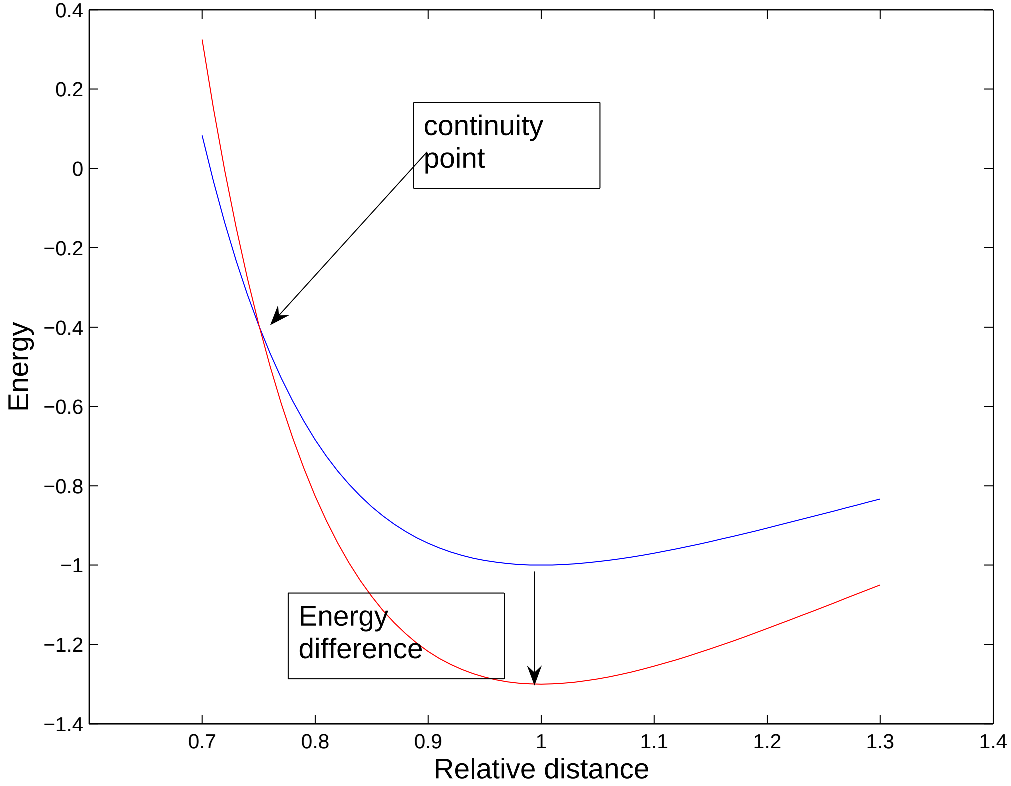
III. Extension to detonation waves

Modeling of detonation in 1D chains

- Important features of detonation:
  - exothermicity (energy release) sustains and enhance the shock wave
  - activation barrier: the speed of the shock wave has to be sufficient for ignition to begin
  - chemical kinetics of the reactions
- Modeling the reaction rate at site n: introduction of an extra variable r_n ($0 \leq r \leq 1$)
- For example, m-th order kinetics (while $r_n \leq 1$)

$$\dot{r}_n = D(1 - r_n)^m$$

Rate-dependent potential



Hardening of the potential + continuity point d_c where chemical reactions are initiated

$$V(d) \rightarrow (1 + Mr)\, V(d) - MV\,(d_c)$$

with r reaction rate, $M > 0$ hardening constant[a]

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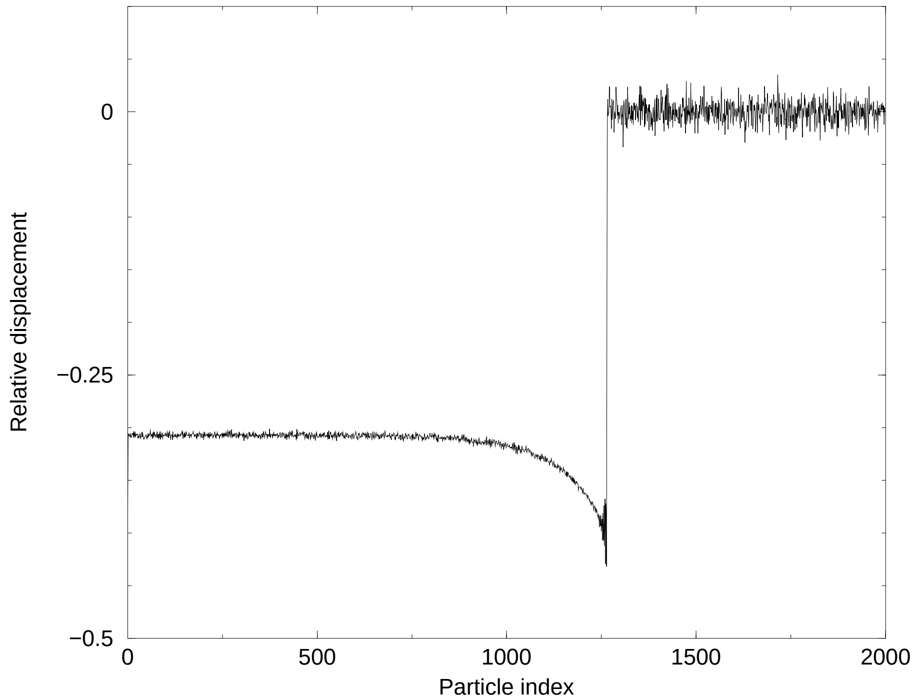
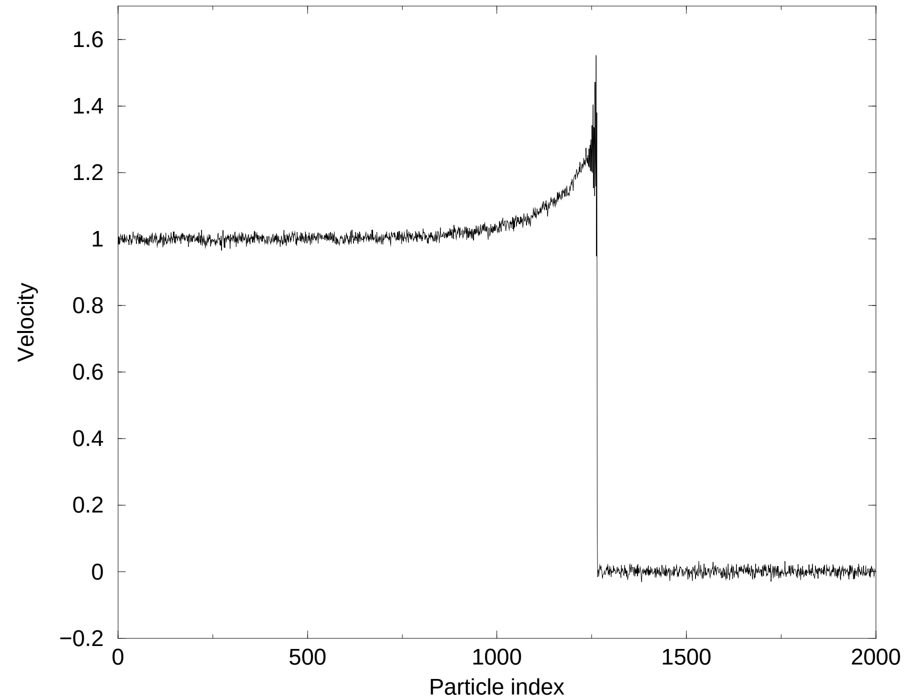
[a]Sornette *et al.* (2003)

Some numerical results





Reactive shock ($K = 1$, first order kinetics $D = 0.025$, $d_c = 0.7$) with the stochastic limit of the harmonic model. Left: Relative displacement profile. Right: Velocity profile.

Some prospects

Some prospects

- Quantitative agreement with real 3D experiments
  - interaction potentials
  - spectrum parameters
  - diatomic chain with next nearest neighbor interactions
- Continuum limit of the model (of the limiting stochastic differential equation)
- Models with reduced degrees of freedom (Holian *et al*) $\longrightarrow$ systematic strategy?