A Simplified One-Dimensional
Shock and Detonation Wa

Gabriel STOLTZ[1,2]

[1] CEA/DAM (Bruyères-le-Châtel, France)

[2] CERMICS, ENPC (Marne-la-Vallée, France)

http://cermics.enpc.fr/∼stoltz/

References

G. Stoltz, *Shock waves in an augmented one-dimensio*
Nonlinearity **18** (2005) 1967-1985

Presentation and preprints available at the URL
`http://cermics.enpc.fr/~stoltz/`

Why looking for a simplified mo

Shock/detonation waves are multiscale phenomena

Different descriptions (fluid dynamics, molecular dynamic

Usually, MD is used to calibrate parameters

A direct micro/macro limit (at least in some asymptotic re very interesting

Hence simplified 1D model since mathematical results o 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-dimer

atom chains

The model

x_{n-1} x_n

Consider the Hamiltonian (nearest-neighbor interactions

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

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

Newton's equations of motion:

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

Usually, Lennard-Jones like potential (possibly Morse or

Normalization conditions $V(0) = 0,\ \ V'(0) = 0,\ \ V''(0) =$

$b = -V'''(0)$ measures at the first order the anharmonicit

Shocks in the 1D chain

- Shock obtained by compression by an infinitely massive
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 c
averaging over several realizations

---

[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 poter
initially at rest. Left: Relative displacement profile ($x_{n+1} - x_n$)
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 potenti
initially at rest. Left: Relative displacement profile ($x_{n+1} - x_n$)
velocity. The sizes of the different regions grow linearly in tim

Thermalized strong shock profil

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

II. Introducing some mean l
dimensional perturbatio

3D is not 1D

1D shocks behave badly because there is no room for re
(formation of the most energetic waves = binary waves)

3D shocks are 1D like only at $T = 0$ and when the compr
along a principal axis[a]

Otherwise, local equilibrium is quickly restored after the s
passed

Idea: the transverse degrees of freedom are necessary f
= thermostat like degrees of freedom!

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

The form of the transverse pertu

y

d_n

x_n θ

Assumption: constrained d.o.f in the tranverse and longitudina
(d.o.f. reduction)
Linearization around equilibrium geometry (FCC <100> struct

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

General case: sum of potentials with different spring constant

The augmented 1D model

System (S) and a heat bath (B) described by bath variab
$(n \in \mathbb{Z},\ j = 1, \ldots, N)$.

The full Hamiltonian reads:

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

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

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

Interpretation: each longitudinal spring length is thermos

Spectrum $\omega_j^2 = k_j$, coupling constants γ_j

Choice of the spectrum parame

Compute the solutions for y, and insert it into the equatio

$$\ddot{x}_n(t) = V'(x_{n+1} - x_n) - V'(x_n - x_{n-1})$$
$$+ \int_0^t K_N(t-s)(\dot{x}_{n+1} - 2\dot{x}_n + \dot{x}_{n-1})(s)$$

σ random forcing term

memory kernel $K_N(t) = \sum_{j=1}^{N} \gamma_j^2 \omega_j^2 \cos(\omega_j t)$ ("generalize equation")

Exponentially decreasing in time ($\mathrm{e}^{-\alpha t}$) in the limit $N \to$

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

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

Some numerical results

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

Some numerical results (2)

Same parameters, but results averaged over 10 realizations.
remain oscillations at the shock front (similar results exist for 3

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

A nonlinear bath model

Thermostating with less tranverse variables and for stron

Model

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

with

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

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

Some numerical results

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

Some numerical results (2)

Same parameters, but results averaged over 100 realizations.

III. Extension to detonation v

Modeling of detonation in 1D ch

Important features of detonation (ZND theory[a]):

- exothermicity (energy release) sustains and enhance
- activation barrier: the speed of the shock wave has to ignition to begin
- chemical kinetics of the reactions

Modeling the reaction rate at site n: introduction of an ex $(0 \leq r \leq 1)$

For example, m-th order kinetics (while $r_n \leq 1$)

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

[a] Fickett and Davis, *Detonation*

Rate-dependent potential

Hardening of the potential + continuity point d_c where chemica
initiated

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

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

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

Some numerical results

Scaling of parameters: $\alpha \to \alpha\sqrt{1 + Kr_n}$ (memory), $\lambda \to \lambda\sqrt{1$
constant)

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

Some prospects

Some prospects

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