Wave of transition in chains and lattices from bistable elements

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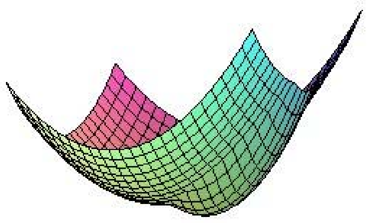
Delft, Dec. 2003

Polymorphic materials



- *Smart materials, martensite alloys, polycrystals* and similar materials can exist in several forms (phases).
- The Gibbs principle states that the phase with minimal energy is realized.

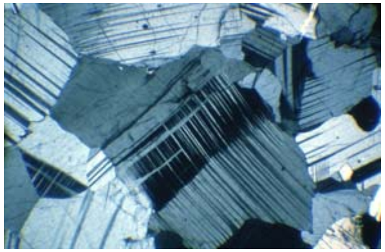
$$\Phi(\nabla w) = \min_{(\chi_1 \ldots \chi_N)} \sum_i \chi_i W_i(\nabla w)$$

W_i is the stable energy of each phase,
χ_i is the characteristic function of the phase layouts,
Φ is the resulting (nonconvex) energy
w is the displacement

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in \Omega_i \\ 0 & \text{if } x \notin \Omega_i \end{cases}$$

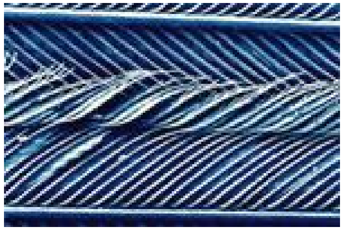
Energy minimization + nonconvexity =structured materials

Martensites alloy with “twin” monocrystals

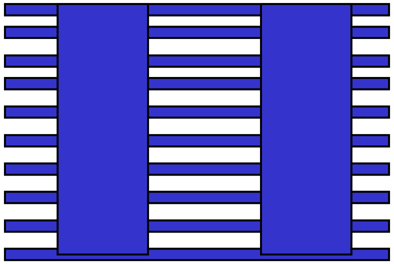


Polycrystals of granulate

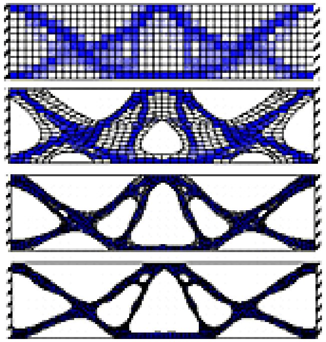
Mozzarella cheese



Falcon’s Feather

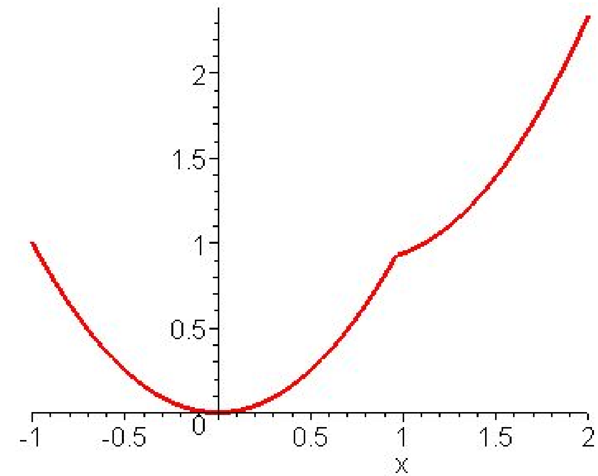


An optimal isotropic conductor



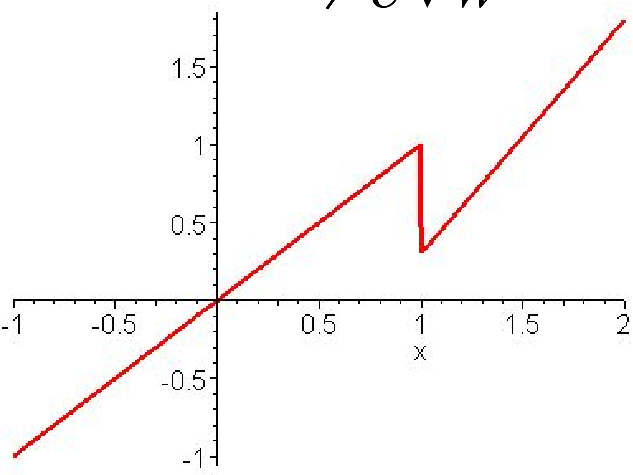
An optimal design

Dynamic problems for multiwell energies



$$\nabla w$$

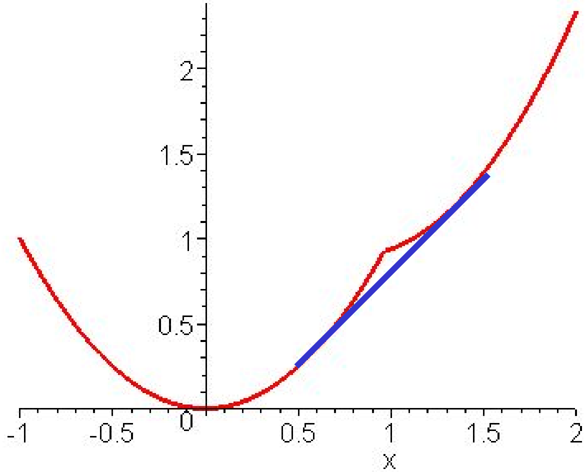
$$\sigma = \partial\Phi \Big/ \partial\nabla w$$



- Problems of description of damageable materials and materials under phase transition deal with nonmonotone constitutive relations

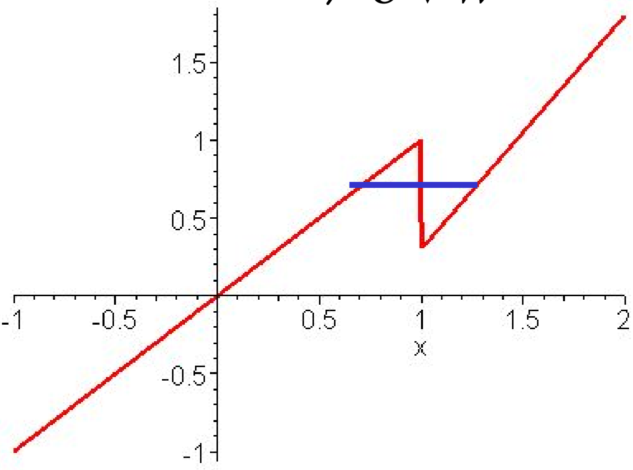
- **Nonconvexity** of the energy leads to **nonmonotonicity** and **nonuniqueness** of constitutive relations.

Static (Variational) approach



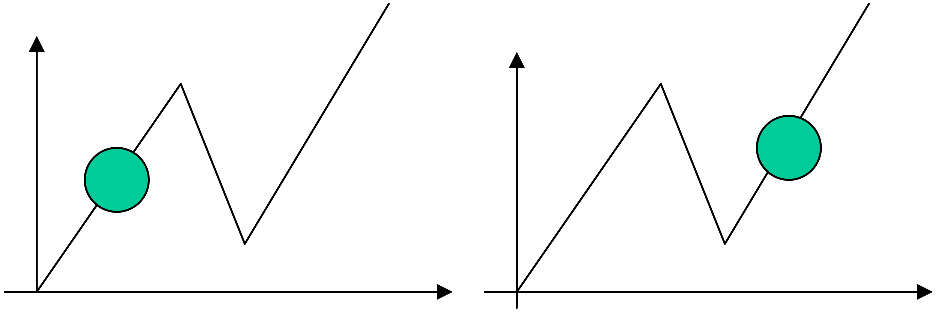
w

$$\sigma = \partial\Phi \big/ \partial\nabla w$$

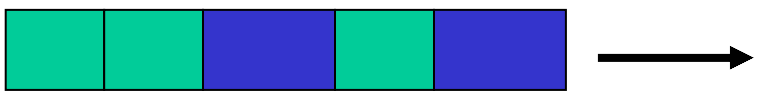


The Gibbs variational principle is able to select the solution with the least energy that corresponds to the (quasi)convex envelope of the energy.

At the micro-level, this solution corresponds to the transition state and results in a fine mixture of several pure phases (Maxwell line)

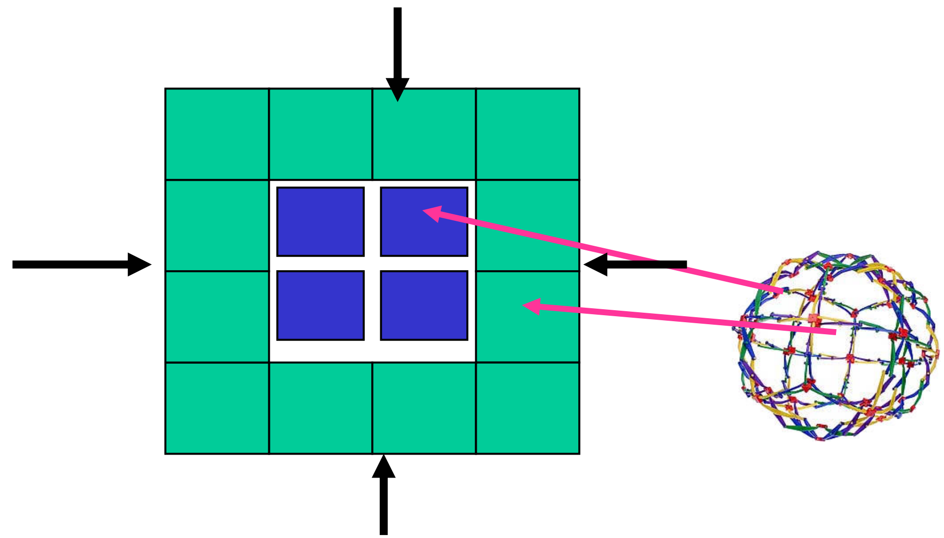


Multivariable problems: Account for integrability conditions leads to quasiconvexity



•One-dimensional problem:

The strain u' in a stretched composed bar can be discontinuous



In multidimensional problems,
the tangential components of the strain
are to be continuous, Correspondingly,
Convexity is replaced with Quasiconvexity

The only possible mode of deformation of an elastic medium is the uniform contraction (Material from Hoberman spheres), then

The strain field is continuous everywhere

Dynamic problems for multiwell energies

- Formulation: Lagrangian for a continuous medium

If W is (quasi)convex $$L(u) = \tfrac{1}{2}\rho\dot{u}^2 - W(\nabla u)$$

- If W is not quasiconvex ~~$L(u) = \tfrac{1}{2}\rho\dot{u}^2 - QW(\nabla u)$~~ ???

$$L(u) = \tfrac{1}{2}\rho\dot{u}^2 - H_D W(\nabla u) - \Theta(u, \dot{u}, \nabla u)$$

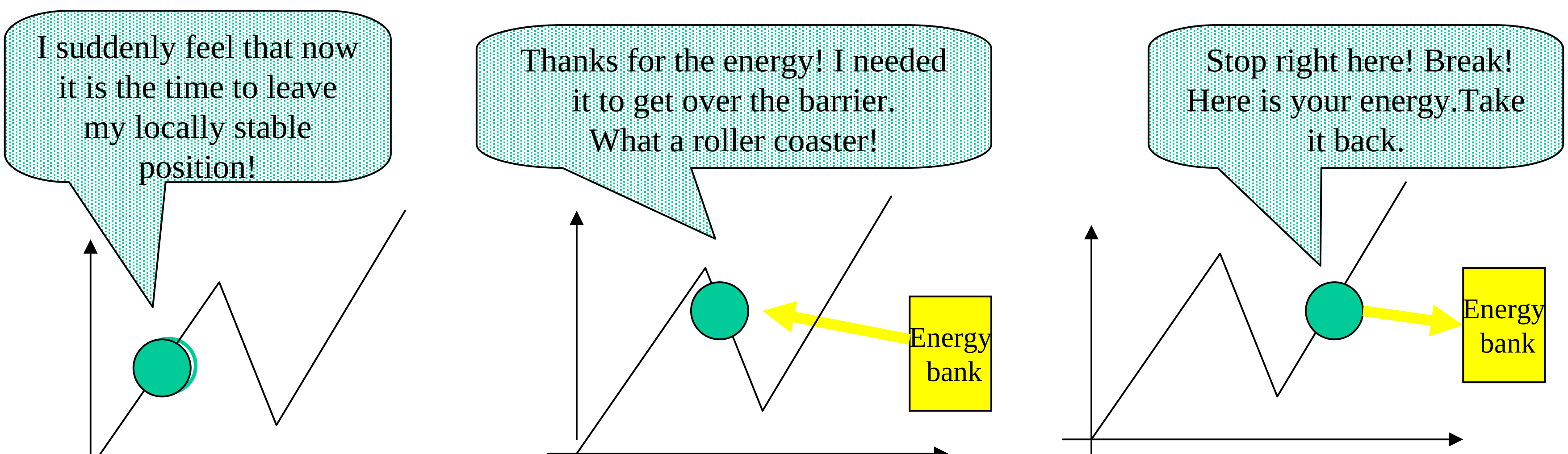
Radiation and other losses

Dynamic homogenization

- Questions:
  - There are many local minima; each corresponds to an equilibrium. How to distinguish them?
  - The realization of a particular local minimum depends on the existence of a path to it. What are initial conditions that lead to a particular local minimum?
  - How to account for dissipation and radiation?

Paradoxes of relaxation of an energy by a (quasi)convex envelope.

- To move along the surface of minimal energy, the particles must:
  - Sensor the proper instance of jump over the barrier
  - Borrow somewhere an additional energy, store it, and use it to jump over the barrier
  - Get to rest at the new position, and return the energy

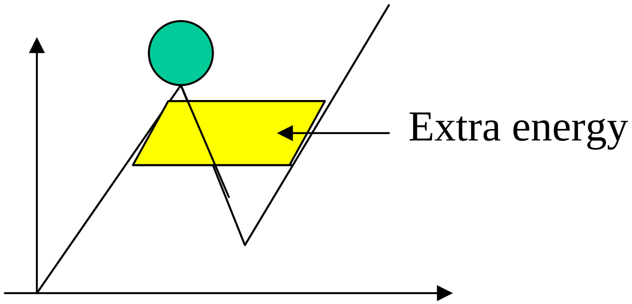


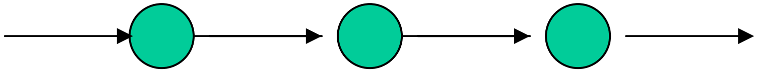
Method of dynamic homogenization

- We are investigating mass-spring chains and lattices, which allows to
  - account for concentrated events as breakage
  - describe the basic mechanics of transition
  - compute the speed of phase transition.
- The atomic system is strongly nonlinear but can be piece-wise linear.
- To obtain the macro-level description, we
  - analyze the solutions of this nonlinear system at micro-level
  - homogenize these solutions,
  - derive the consistent equations for a homogenized system.

Waves in active materials

- Links store additional energy remaining stable. Particles are inertial.
- When an instability develops, the excessive energy is transmitted to the next particle, originating the wave.
- Kinetic energy of excited waves takes away the energy, the transition looks like an **explosion.**
- Active materials: Kinetic energy is **bounded from below**
- Homogenization: Accounting for radiation and the energy of high-frequency modes is needed.





Dynamics of chains from bi-stable elements (exciters)

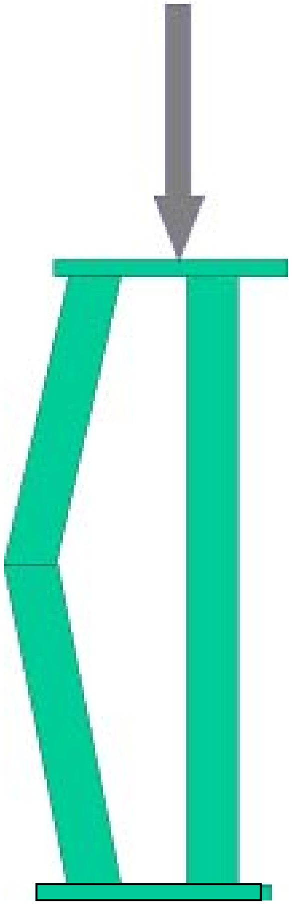
with Alexander Balk, Leonid Slepyan, and Toshio Yoshikawa

A.Balk, A.Cherkaev, L.Slepyan 2000. IJPMS

T.Yoshikawa, 2002, submitted

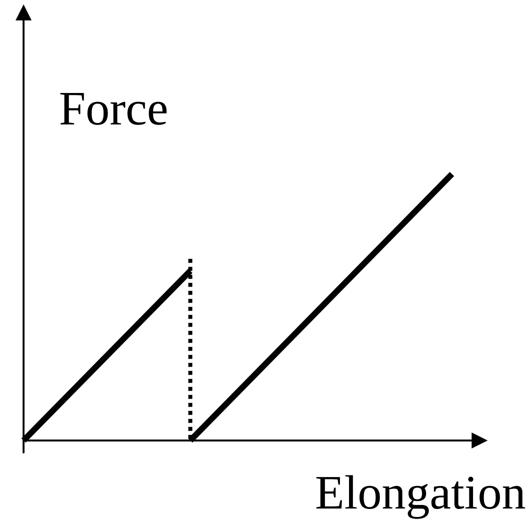
Delft, Dec. 2003

Unstable reversible links



- Each link consists of two parallel elastic rods, one of which is longer.
- Initially, only the longer road resists the load.
- If the load is larger than a critical (buckling)value:
  - ✓ The longer bar looses stability (buckling), and
  - ✓ the shorter bar assumes the load.

The process is reversible.



$$f(x) = x - H(x-1)$$

H is the Heaviside function

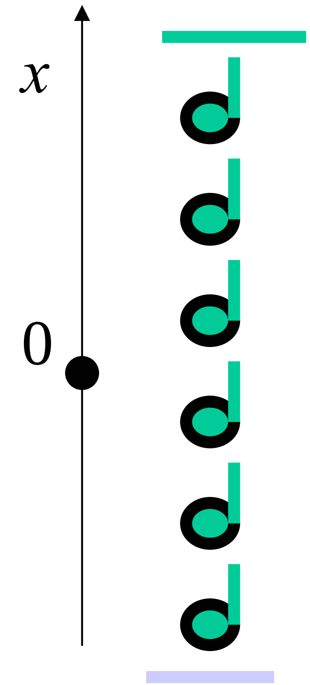
No parameters!

Chain dynamics. Generation of a spontaneous transition wave

$$m\ddot{X}_k = f(X_k - X_{k-1}) - f(X_{k+1} - X_k) = L(X_k) + N(X_k)$$

$$L(X_k) = \underbrace{X_{k-1} - 2X_k + X_{k+1}}_{\text{linear chain}}$$

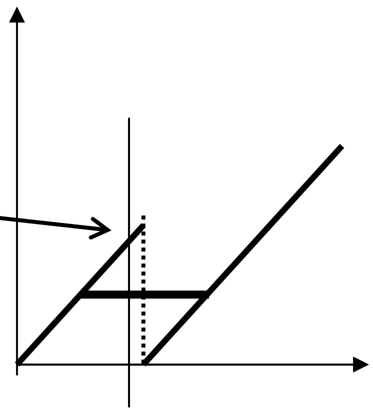
$$N(X_k) = \underbrace{H(X_k - X_{k-1} - a) - H(X_{k+1} - X_k - a)}_{\text{nonlinear impacts}}$$



Initial position:

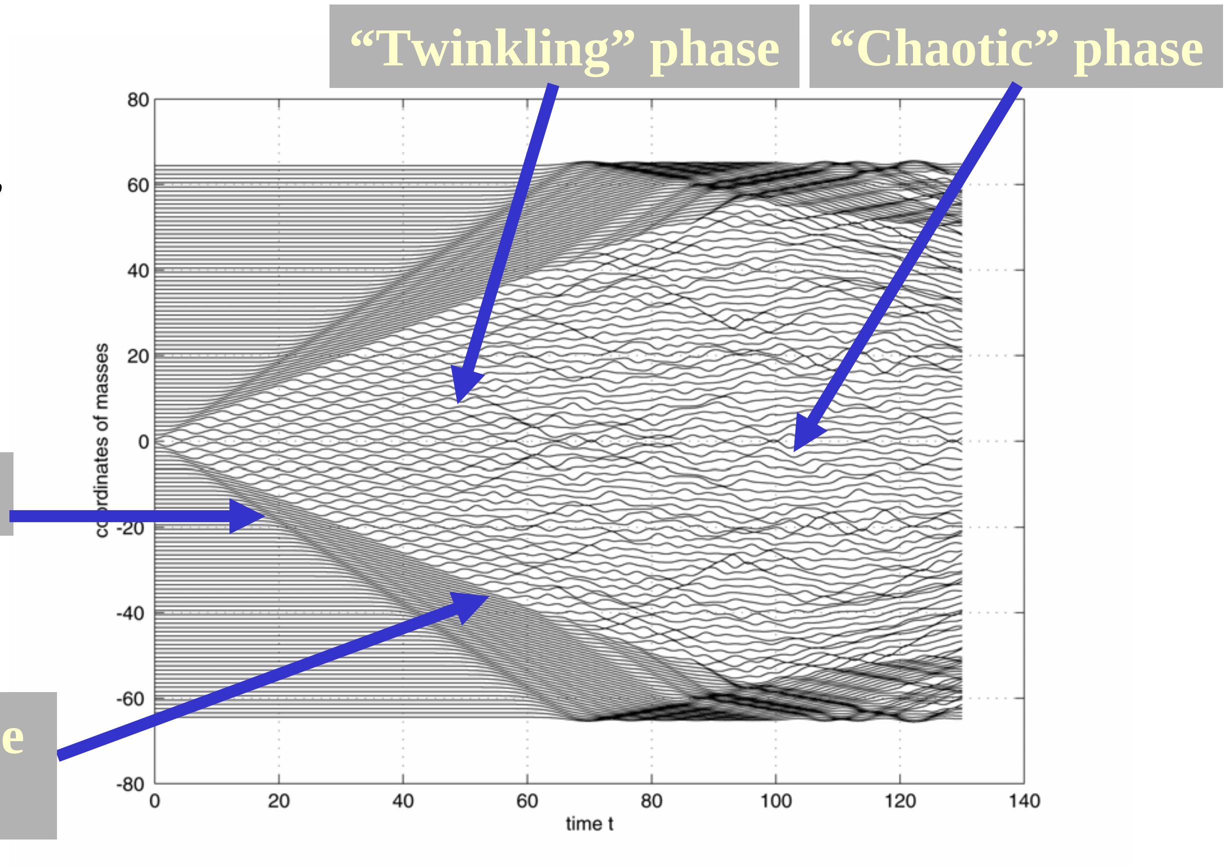
$$x_k = (a - 1 - \varepsilon)k$$

(linear regime, close to the critical point)

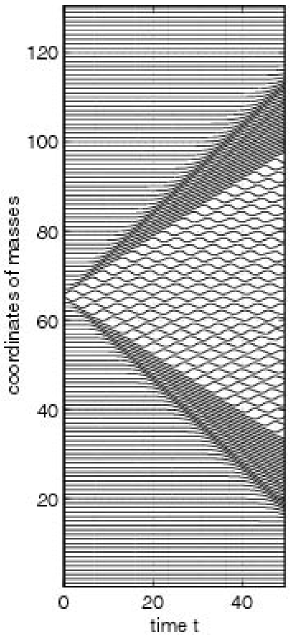


Observed spontaneous waves in a chain

Under a smooth excitation, the chain develops intensive oscillations and waves.



“Twinkling” phase and Wave of phase transition (Small time scale)



$$m\ddot{X}_k = f(X_k - X_{k-1}) - f(X_{k+1} - X_k) = L(X_k) + N(X_k)$$

$$L(X_k) = \underbrace{X_{k-1} - 2X_k + X_{k+1}}_{\text{linear chain}}$$

$$N(X_k) = \underbrace{H(X_k - X_{k-1} - a) - H(X_{k+1} - X_k - a)}_{\text{nonlinear impacts}}$$

After the wave of transition, the chain transit to a new twinkling (or headed) state.

We find global (homogenized) parameters of transition:

- ✓ Speed of the wave of phase transition
- ✓ “Swelling” parameter
- ✓ Period
- ✓ Phase shift

Periodic waves: Analytic integration

Approach, after Slepyan and Troyankina

$$\tilde{N}(t) = H(\sin(\omega t + p)) - H(\sin(\omega t - p));$$ → Nonlinearities are replaced by a periodic external forces; period is unknown

$$X_k(t) = X_{k-1}(t - \tau) + a;$$ → Self-similarity

$$X_k(t) = X_k(t + 2\pi\omega);$$ → Periodicity

$$\left.\begin{aligned} m\ \ddot{x}(t) &= x(t+\tau) - 2x(t) + x(t-\tau) \\ &+ H_T(t+\theta) - H_T(t+T-\theta) \end{aligned}\right\} (*)$$

System (*) can be integrated by means of Fourier series.

A single nonlinear algebraic equation defines the instance θ.

1. Stationary waves

Use of the piece-wise linearity of the system of ODE and the above assumptions

The system is integrated as a linear system (using the Fourier transform),

$$\left(p^2 + 4\sin^2(p\tau)\right)\overline{X}(p) = \frac{e^{p\theta} - e^{p(\omega-\theta)}}{1 - e^{p\omega}} \qquad X(t) = F^{-1}\overline{X}(p)$$

then the nonlinear algebraic equation

$$X(t) - X(t+\theta) = 1$$

for the unknown instances θ of the application/release of the applied forces is solved.

Result: The dispersion relation

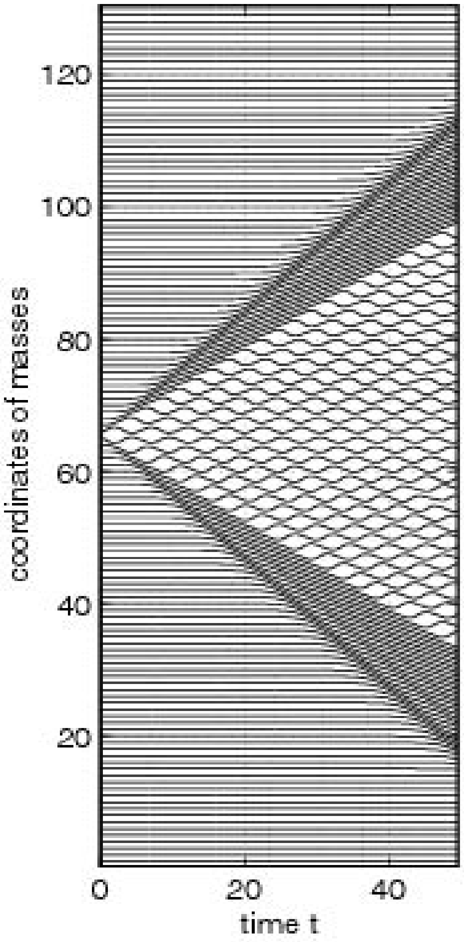
2. Waves excited by a point source

For the wave of phase transition we assume that ***k***-th mass enters the twinkling phase after ***k*** periods

$$\tilde{\tilde{N}}_k(t) = \begin{cases} \tilde{N}_k(t), \text{ if } t > 2\pi\omega k, \\ 0, \qquad \text{otherwise} \end{cases}$$

The self-similarity assumption is weakened.

Asymptotic periodicity is requested.



Large time range description

with Toshio Yoshikawa

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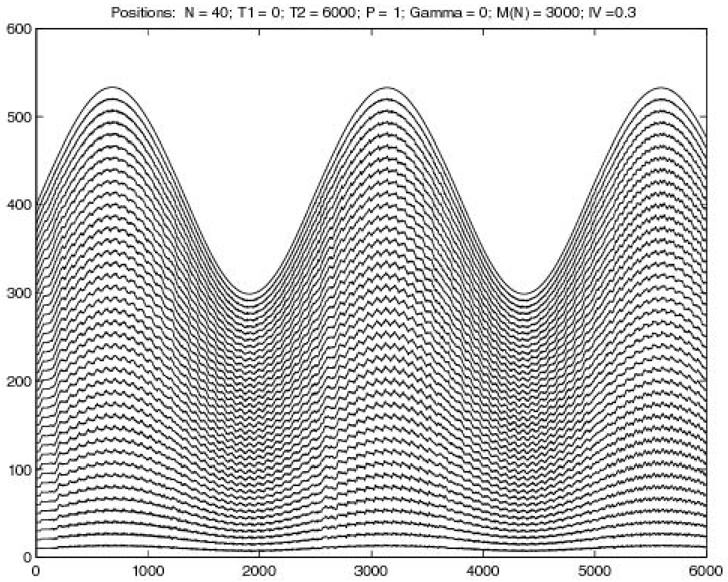
Problem of dynamic homogenization

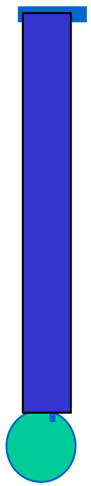


Consider a chain, fixed at the lower end and is attached by a “heavy” mass ***M=3,000 m*** at the top.

$$m\ddot{x}_k = f(x_{k+1} - x_k - a) - f(x_k - x_{k-1} - a), k = 1, \dots, N-1,$$

$$M\ddot{x}_N = -f(x_N - x_{N-1} - a), \quad x_0 = 0.$$

T >> 1/M, M >>m



Problem:

Approximate the motion of the mass ***M*** by a single differential equation

$$M\ddot{L} = \Psi(L), \quad L = \sum X_k,$$

Find $\Psi(L)$

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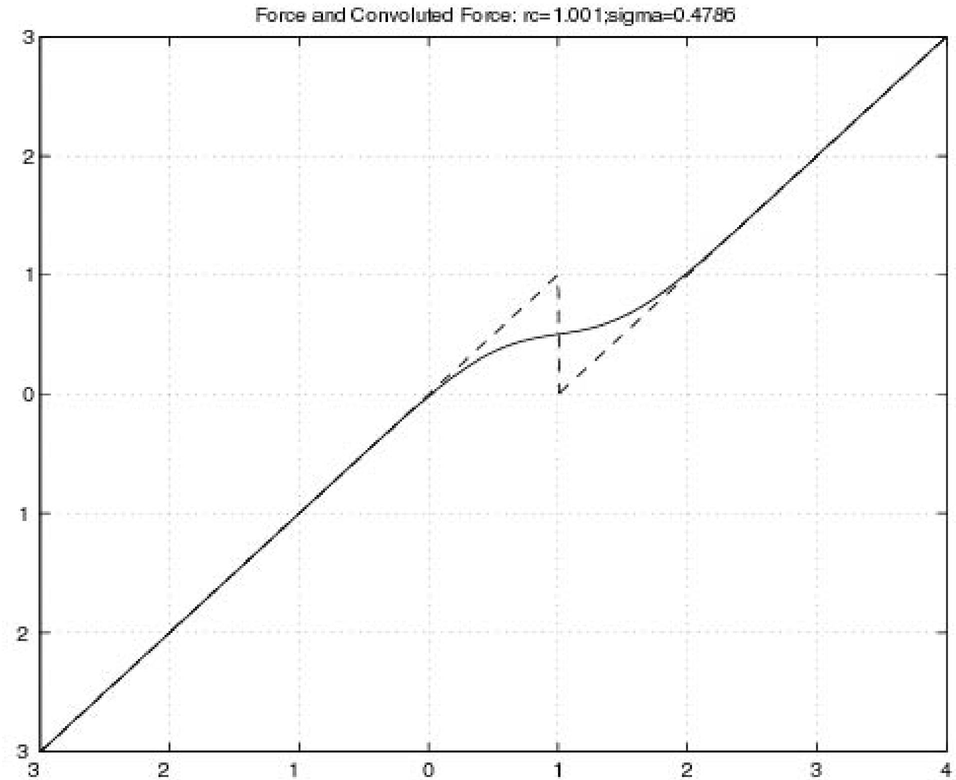
Result: numerics + averaging

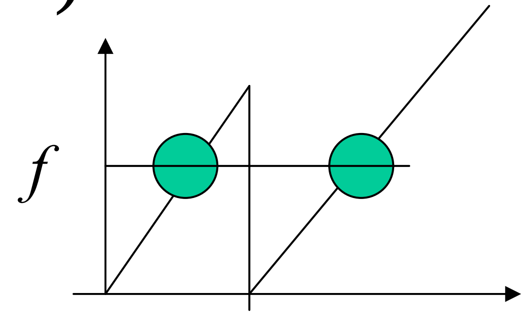
Average curve is smooth and monotonic.

Minimal value of derivative is close to zero.



Homogenized constitutive relation (probabilistic approach)

$$\psi_k = F^{-1}p(f) + (F^{-1} + \Delta)(1 - p(f))$$



Coordinate of the “large mass” is the sum of elongations of many nonconvex springs that (as we have checked by numerical experiments) are almost uncorrelated, (the correlation decays exponentially,) while the time average of the force is the same in all springs:

$$\Psi^{-1}(f) = F^{-1}(f) + \operatorname{erf}\left(\frac{f - f_0}{\sigma}\right), \quad E = \Delta = 1.$$

The dispersion is of the order of the hollow in the nonconvex constitutive relation.

Add a small dissipation:

$$m\ddot{X}_k + \alpha\dot{X}_k = f(X_k - X_{k-1}) - f(X_{k+1} - X_k)$$

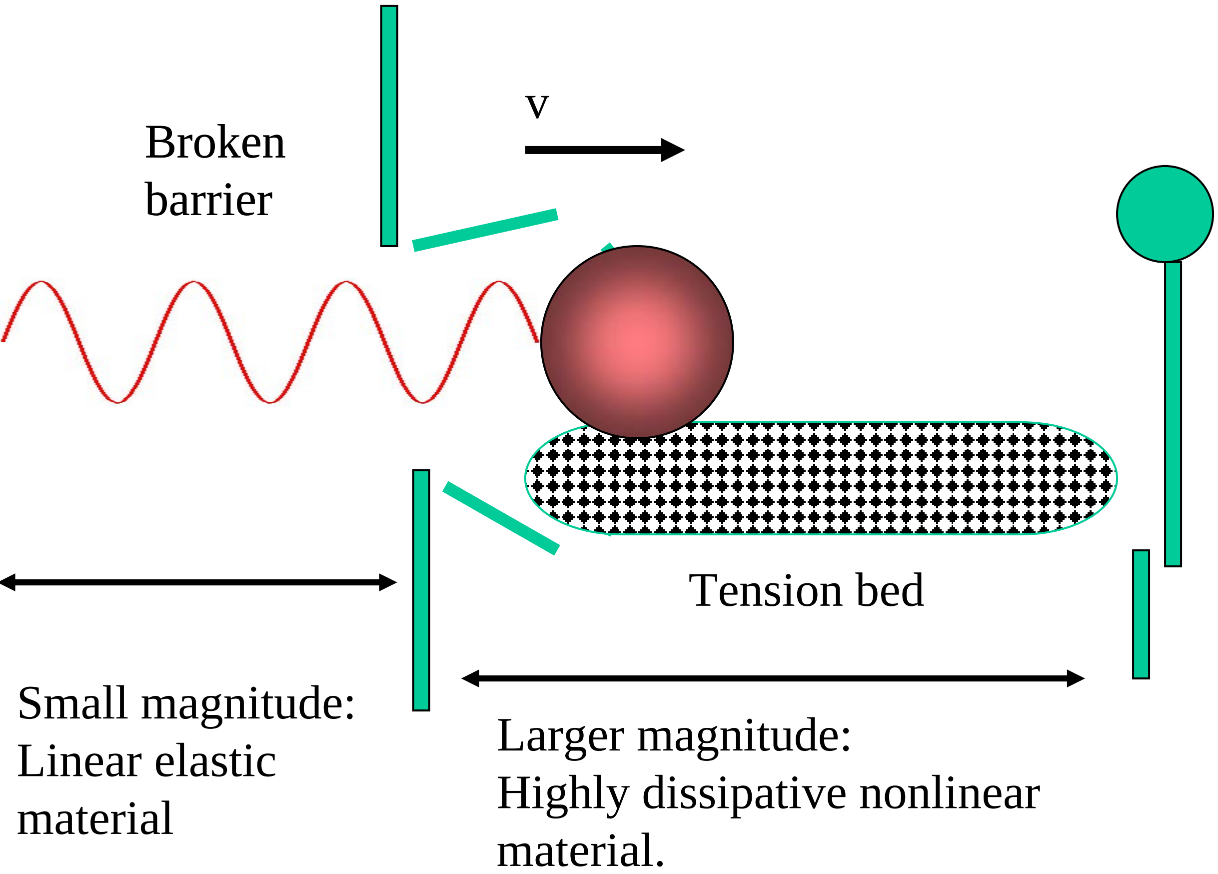
Continuous limit is very different: The force becomes

$$\Psi \cong k\,\mathrm{sign}(\dot{x}),\ \text{if}\ x \in [x_l, x_u]$$

$$\Psi \cong f(x), \quad \text{if}\ x \notin [x_l, x_u]$$

The system demonstrates a strong hysteresis.

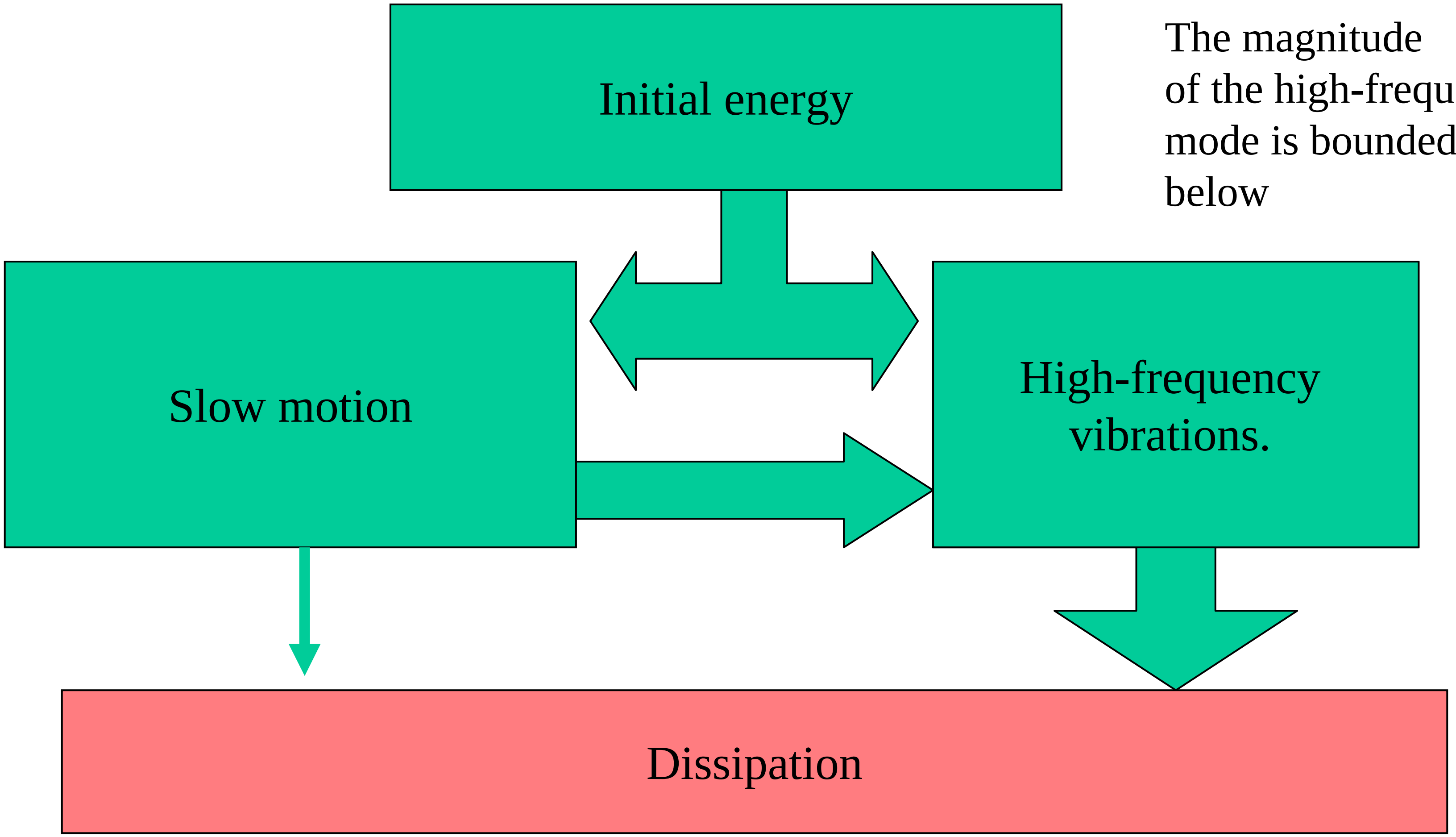
Homogenized model (with dissipation)



- Initiation of vibration is modeled by the break of a barrier **each time** when the unstable zone is entered.
- Dissipation is modeled by tension in the unstable zone.

Energy path

The magnitude
of the high-frequency
mode is bounded from
below



Waves in infinite bistable chains (irreversible transition)

In collaboration with Elena Cherkaev, Leonid Slepyan, and Liya Zhornitskaya

Delft, Dec. 2003

Elastic-brittle material (limited strength)

- The force-versus-elongation relation is a monotonically elongated bar from elastic-brittle material is

$$f(x) = \begin{cases} Ex, & \text{if } x < x_f \\ 0, & \text{if } x < x_f \end{cases}$$

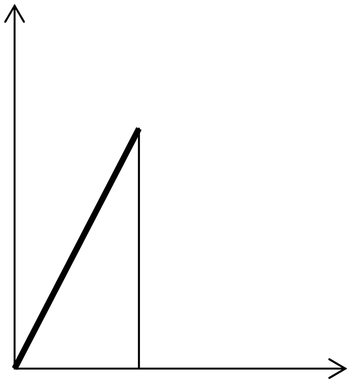
- Accounting for the prehistory, we obtain the relation

$$f(x,t) = Ex(1 - c(x,t)),$$

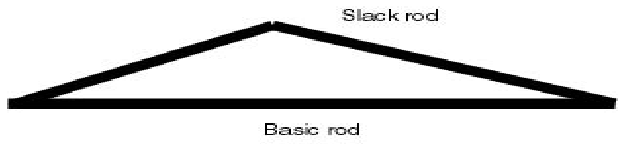
$$\dot{c}(x,t) = \begin{cases} 1 \text{ if } & x > x_f,\, c < 1 \\ 0, & \text{otherwise} \end{cases}$$

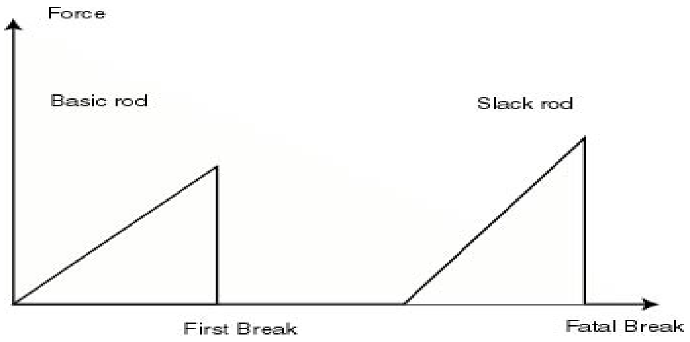
$$c(x,0) = 0$$

c(x,t) is the damage parameter



Waiting links





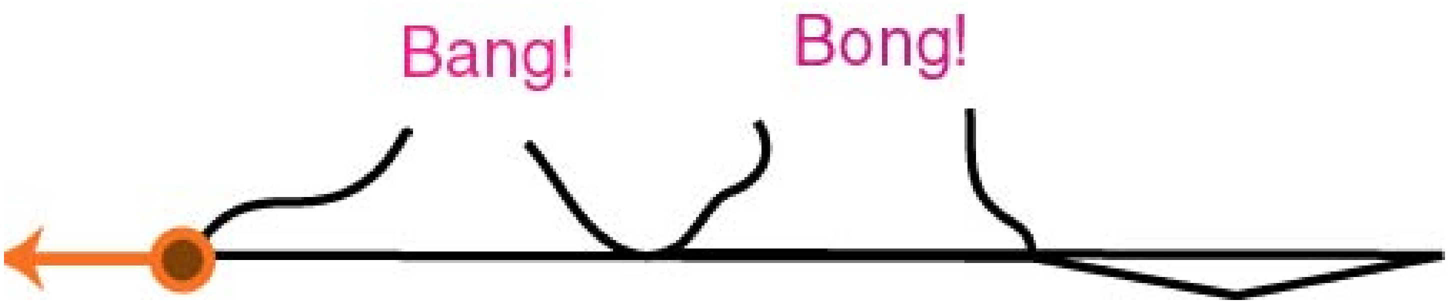
- It consists of two “parallel” rods; one is slightly longer.
- The second (slack) rod starts to resist when the elongation is large enough.
- Waiting links allow to increase the interval of stability.

$$f(L,c_1,c_2) = (1-c_1(L))f_1(L) + (1-c_2(L-\tau))f_2(L-\tau)H(L-\tau)$$

Chain of rods

- Several elements form a chain $m\ddot{x}_k = f(x_{k+1} - x_k - a, c_k) - f(x_k - x_{k-1} - a, c_{k-1})$

What happens when the chain is elongated?



Multiple breakings occur and “Partial damage” propagates along the rod.

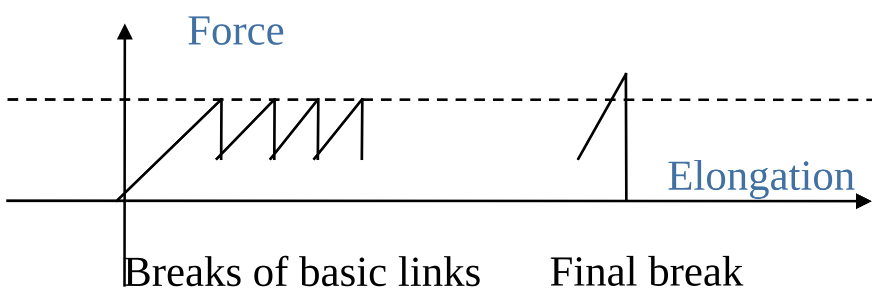
Tao of Damage

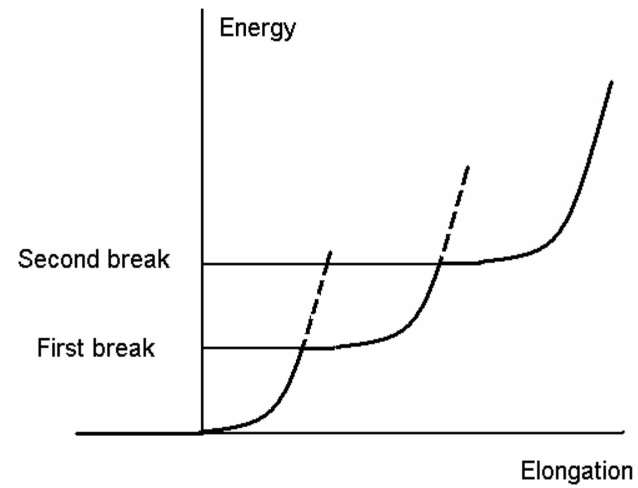
Tao -- the process of nature by which all things change
and which is to be followed for a life of harmony. *Webster*

- Damage happens!
- Uncontrolled, damage concentrates and destroys
- Dispersed damage absorbs energy

- Design is the art of scattering the damage

Quasistratic state and the energy





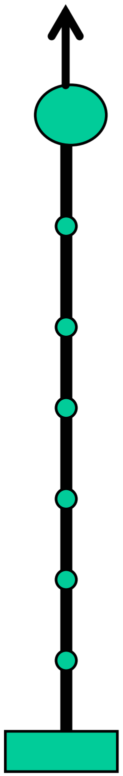
The chain behaves as a superplastic material

The absorbed energy $\boldsymbol{E_w}$ is proportional to the number of “partially damaged” links;

$$\frac{E_w}{E} = 1 + (N - 1)\alpha > 1$$

The chain absorbs more energy before total breakage than a single rod of the combined thickness;

Waves in waiting-link structures



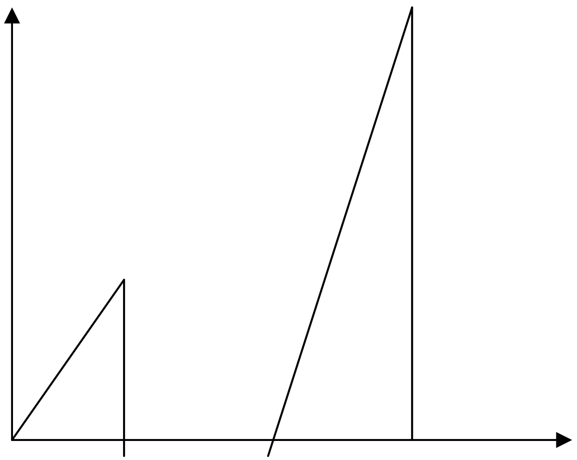
- Breakages transform the energy of the impact to energy of waves which in turn radiate and dissipate it.
- Waves take the energy away from the zone of contact.
- Waves concentrate stress that may destroy the element.

A large slow-moving mass (7% of the speed of sound) is attached to one end of the chain, the other end is fixed.

During the simulation, the mass of the projectile M was increased until the chain was broken.

Constitutive relation

$$m\,\ddot{x}_k + (\gamma\,\dot{x}_k) = f(x_{k+1} - x_k - a) - f(x_k - x_{k-1} - a)$$
$$M\,\ddot{x}_N + (\gamma\,\dot{x}_N) = -f(x_{Nk} - x_{N-1} - a)$$
$$\dot{x}_N(0) = v,\ \dot{x}_k(0) = 0,\ k = 1,\ldots,N-1.$$
$$f(L) = (1-c)f(L) + cf(L-\tau)H(L-\tau)$$

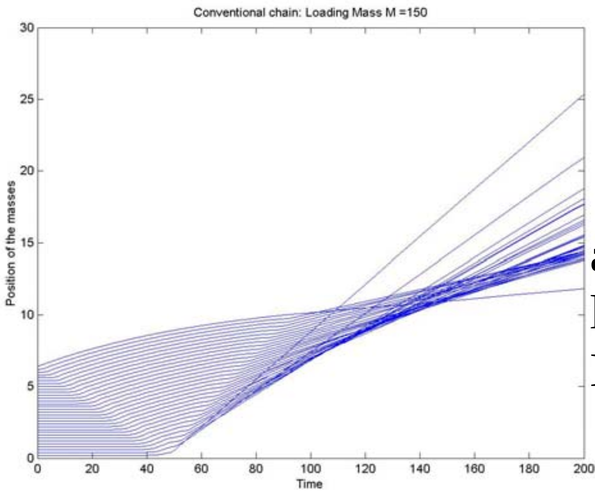


Constitutive relation in links

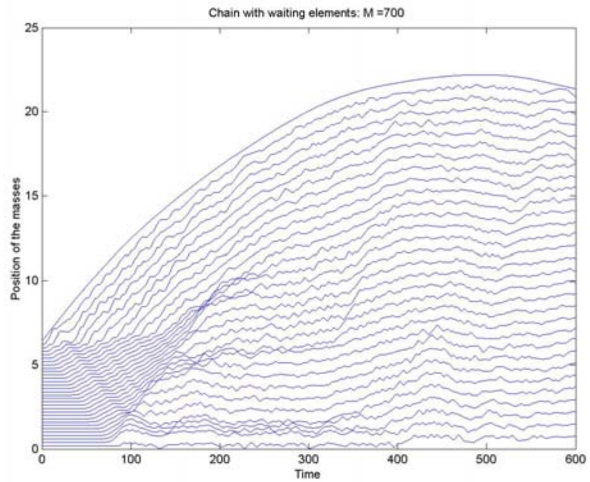
a is the fraction of material
Used in the foreran “basic link

Results

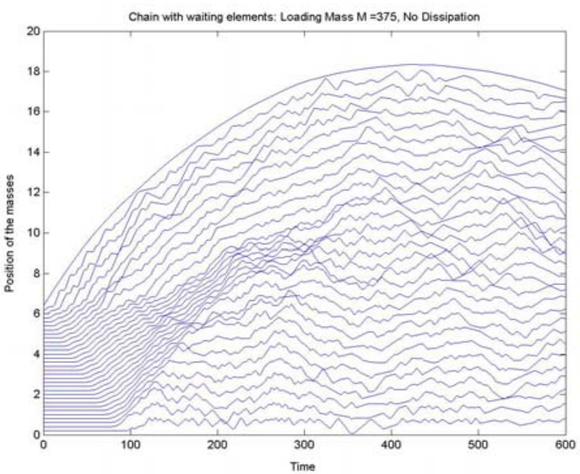
Efficiency: 750/150=5



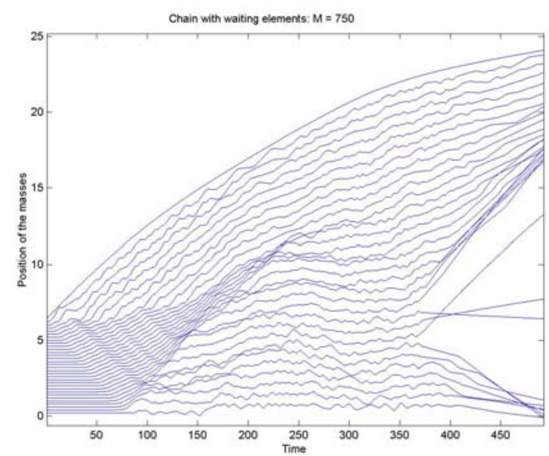
a=1 (no waiting links)
M = 150



M=700
a=.25
Small dissipation



M=375,
a=0.25

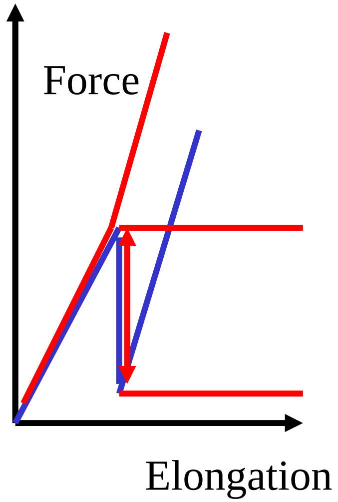


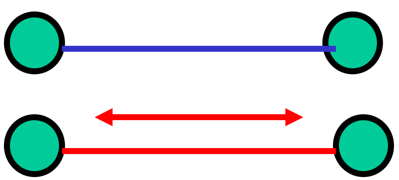
M=750
a=.25
Small dissipation

Use of a linear theory for description of nonlinear chains

The force in a damageable link is viewed as a linear response to the elongation plus an additional external pair of forces, applied in the proper time when Z reaches the critical value.

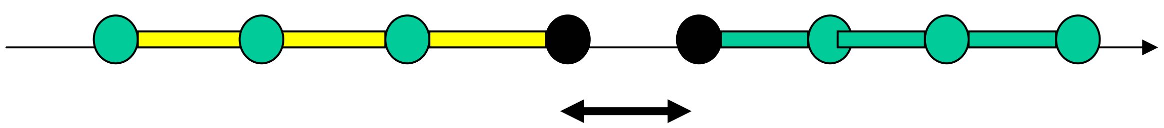
Trick (Slepyan and Troyankina, 1978): model the jump in resistance by an action of an external pair of forces





$$F_{real}(z) = Cz - \beta(z - z_0)$$

$$F_{\mathrm{mod}}(z) = Cz - \beta\, H(t - t_0)$$



Wave motion: Assumptions

- Wave propagate with a constant but unknown speed v
- Motion of all masses is self-similar

$$x_n(t) = x_{n-1}(t - v) + a$$

$$z_n(t) = z_{n-1}(t - v) \quad \text{where} \quad z_n = x_n - x_{n-1}$$

- Therefore, the external pairs of forces are applied at equally-distanced instances

$$t_n = t_{n-1} + v$$

- The problem becomes a problem about a wave in a linear chain caused by applied pair of forces.

Scheme of solution

- Pass to coordinates moving with the wave

$$m\ddot{z} + C(z(t+v) - 2z(t) + z(t-v)) = \gamma[H(t+v) - 2H(t) + H(t-v)]$$

- Using Fourier transform, solve the equation

$$L(p)z^F = G(p);\ G(p) = \cos(pv) - 2,\quad L(p) = -mp^2 + C(\cos(pv) - 2).$$

$$z = \mathsf{F}^{-1}\left[L(p)^{-1}G(p)\right] = z(t,v)$$

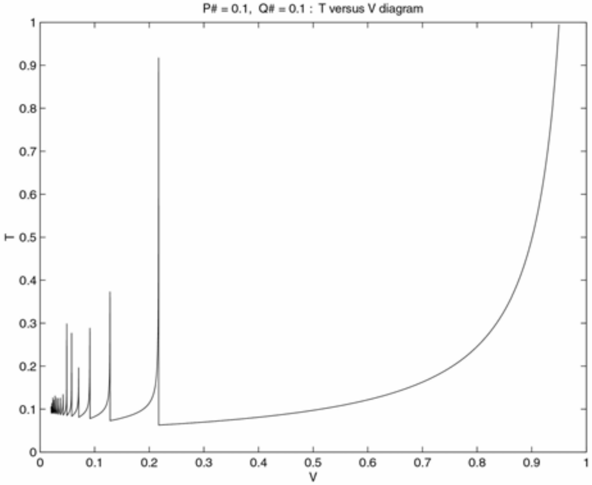
- Return to originals, find the unknown speed from the breakage condition.

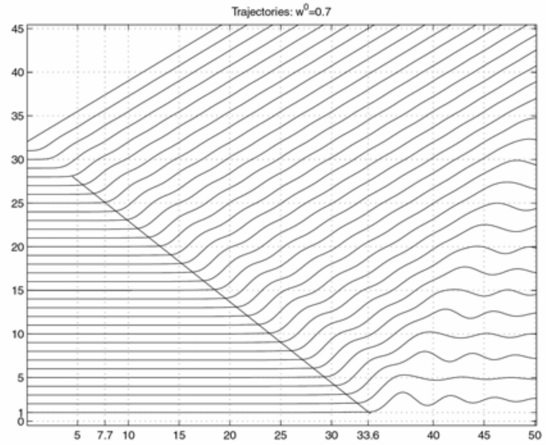
$$z(0,v) = z(1,v)$$

Results

- Dependence of the waves speed versus initial pre-stress *v=v(p)*.

Measurements of the speed





The speed of the wave is found from atomistic model, as a function of prestress.

The propagation of the wave is contingent on its accidental initiation.

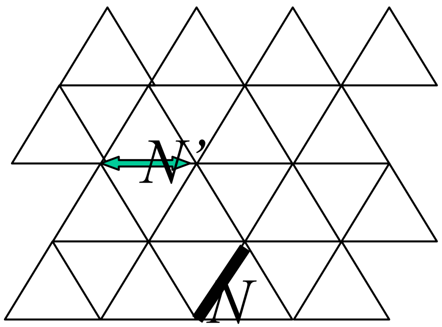
Comments

- The solution is more complex when the elastic properties are changed after the transition.
- One needs to separate waves originated by breakage from other possible waves in the system. For this, we use the “causality principle” (Slepyan) or viscous solutions.
- In finite networks, the reflection of the wave in critical since the magnitude doubles.
- The damage waves in two-dimensional lattices is described in the same manner, as long as the speed of the wave is constant.
- The “house of cards” problem: Will the damage propagate?
- Similar technique addresses damage of elastic-plastic chains.

Lattices with waiting elements

Delft, Dec. 2003

Green’s function for a damaged lattice



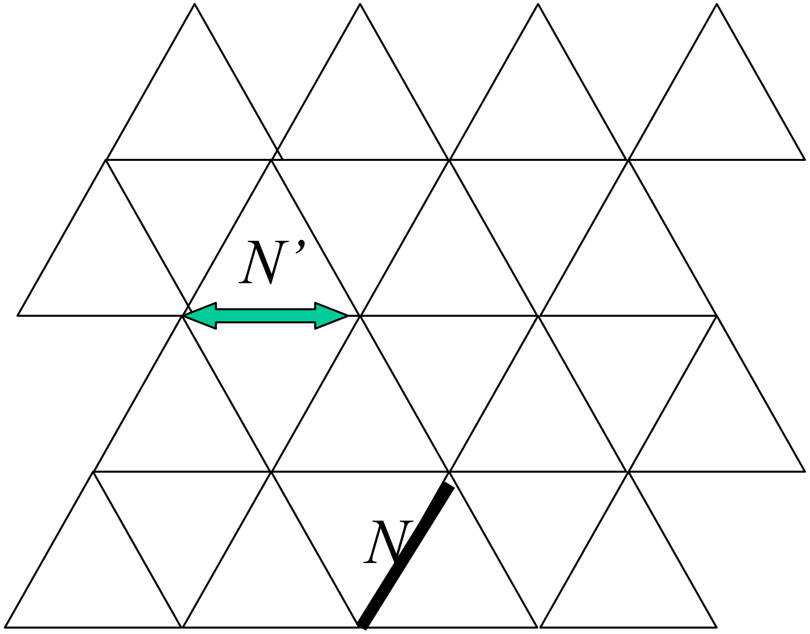
Green’s function: Influence of one damaged link:

$$F(k,m,N,N') =$$
$$G(k-k',m-m') : N \otimes N'$$

F(k,m, N, N’)

$$G^F = \begin{pmatrix} \frac{1}{2}\left(\cos q + \cos(p-q) + 4\cos p - 6\right) & \frac{\sqrt{3}}{2}\left(\cos q - \cos(p-q)\right) \\ \frac{\sqrt{3}}{2}\left(\cos q - \cos(p-q)\right) & \frac{3}{2}\left(\cos q + \cos(p-q) - 2\right) \end{pmatrix}$$

State of a damaged lattice



F(k,m, N, N')

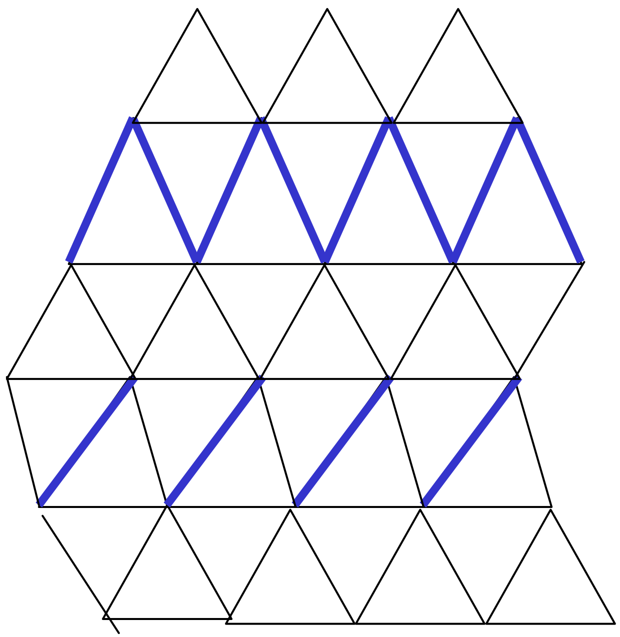
State of a partially damaged lattice:

$$F_{\text{damage}}(k,m,N) = \sum_i G(k-k_i, m-m_i) : N \otimes N_i + F_{\text{extern}}$$

$$F_{\text{damage}}(k,m,N) < TH \quad \forall k,m.$$

Q: How to pass from one permissible configuration to another?

Unstrained damaged configurations

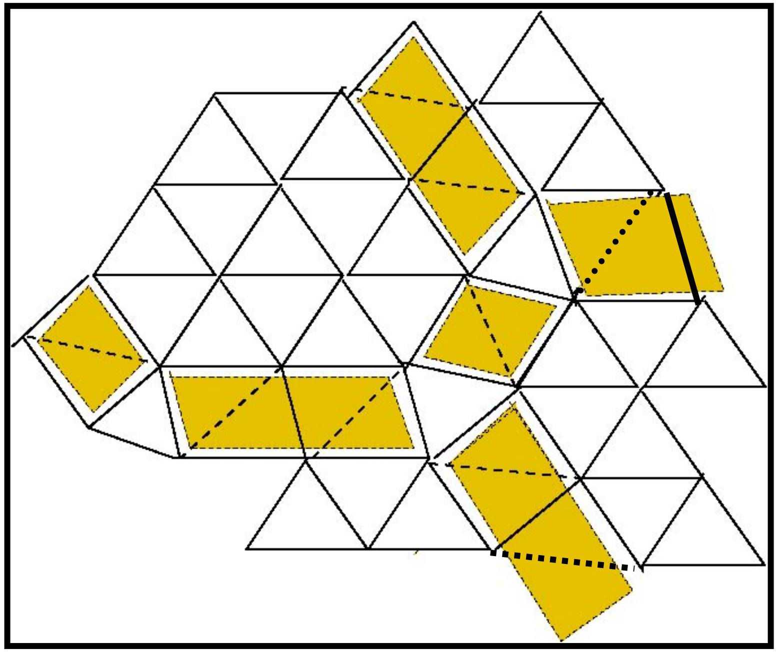


- Generally, damage propagates like a crack due to local stress concentration.
- The expanded configurations are not unique.
- There are exceptional ***unstrained*** configurations

$$F_{\mathrm{damage}}(k,m,N)=0$$

which are the attraction points of the damage dynamics and the null-space of F.

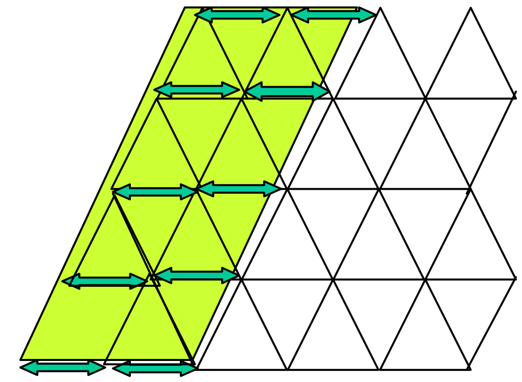
Set of unstrained configurations

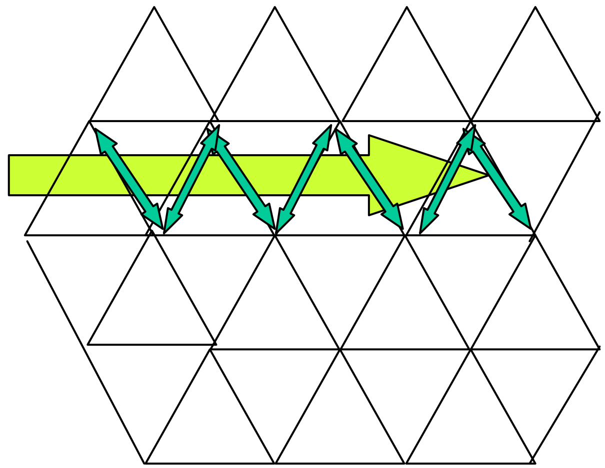


- The geometrical problem of description of all possible unstrained configuration is still unsolved.
- Some sophisticated configurations can be found.
- Because of nonuniqueness, the expansion problem requires dynamic consideration.

Random lattices: Nothing known

Waves in bistable lattices





Today, we can analytically describe two types of waves in bistable triangular lattices:

- Plane (frontal) waves
- Crack-like (finger) waves

We find condition (pre-stress) for the wave propagation and the wave' speed (dispersion relations)

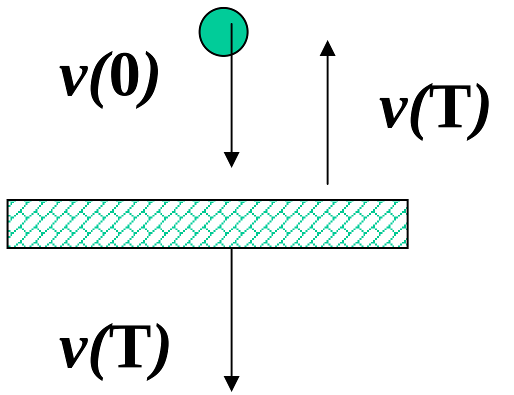
Damage in two-dimensional lattice

(with Liya Zhornitzkaya)

Delft, Dec. 2003

Effectiveness of structure resistance

- To measure the effectiveness, we use the ratio *R* of the momentum of the projectile after and before the impact. This parameter is independent of the type of structural damage.



Elastic collision	Free propagation	rejection	absorption
Value of R	1	-1	0

Conclusion

- The use of atomistic models is essential to describe phase transition and breakable structures.
- These models allows for description of nonlinear waves, their speed, shape change, and for the state of new twinkling phase.
- Dissipation is magnified due to accompanied fast oscillations.
- Radiation and the energy loss is described as activation of fast modes.