WAVES IN MATERIALS WITH MICROSTRUCTURE: NUMERICAL SIMULATION

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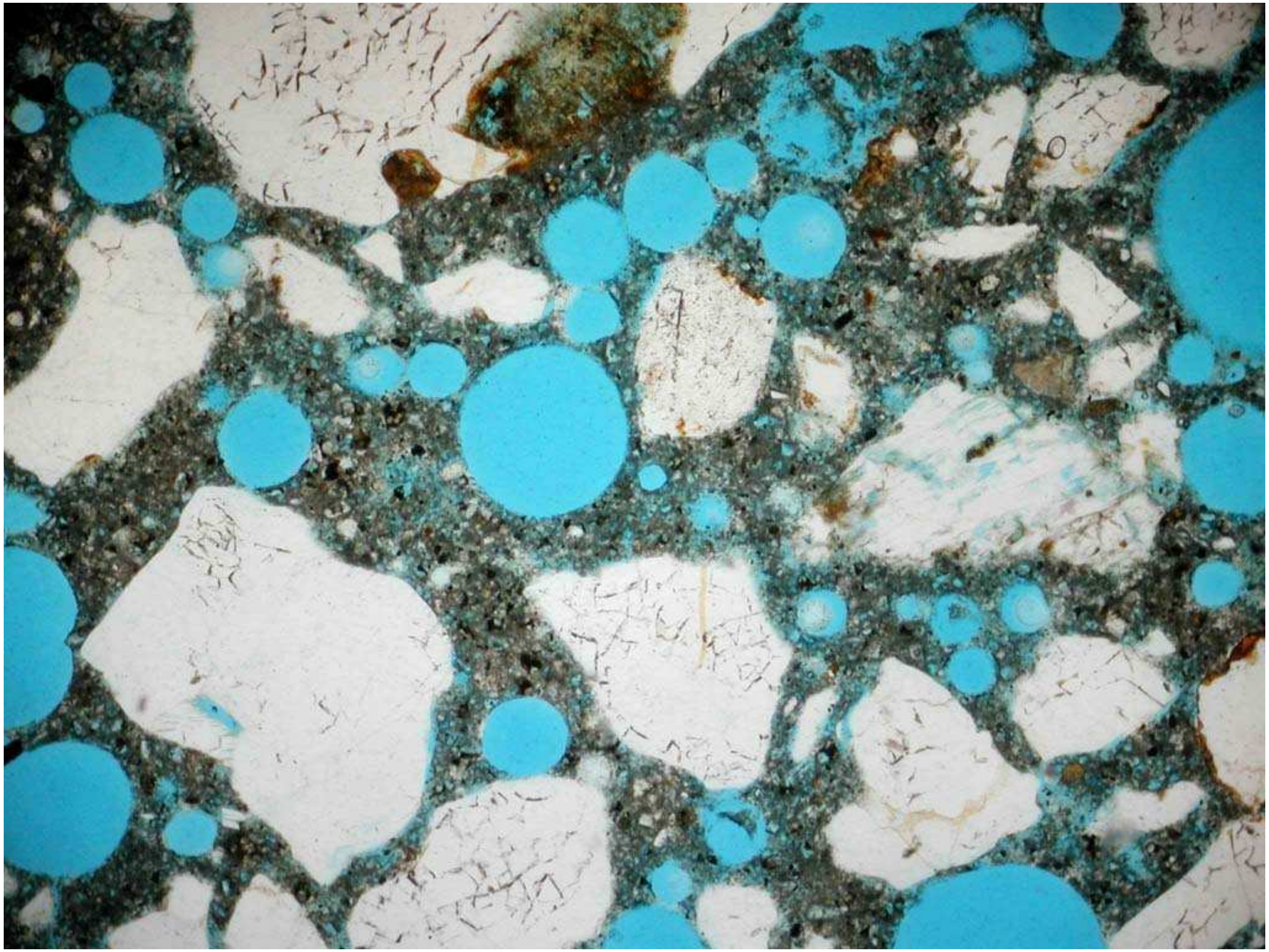
Outline

- Motivation
- Microstructure model
  - Dual internal variables approach
  - Balance laws
- Numerical results
- Conclusion

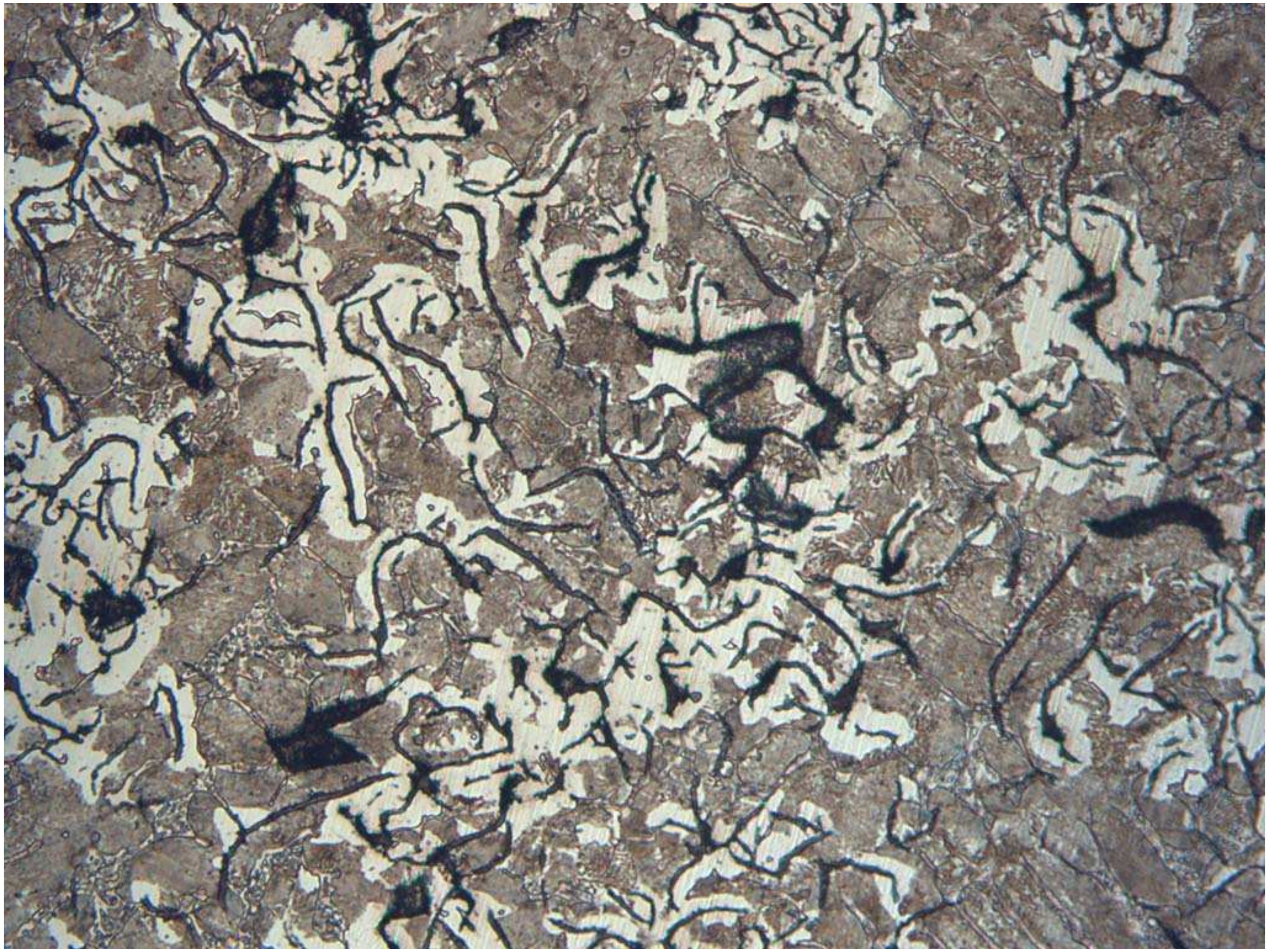
Motivation

Microstructure



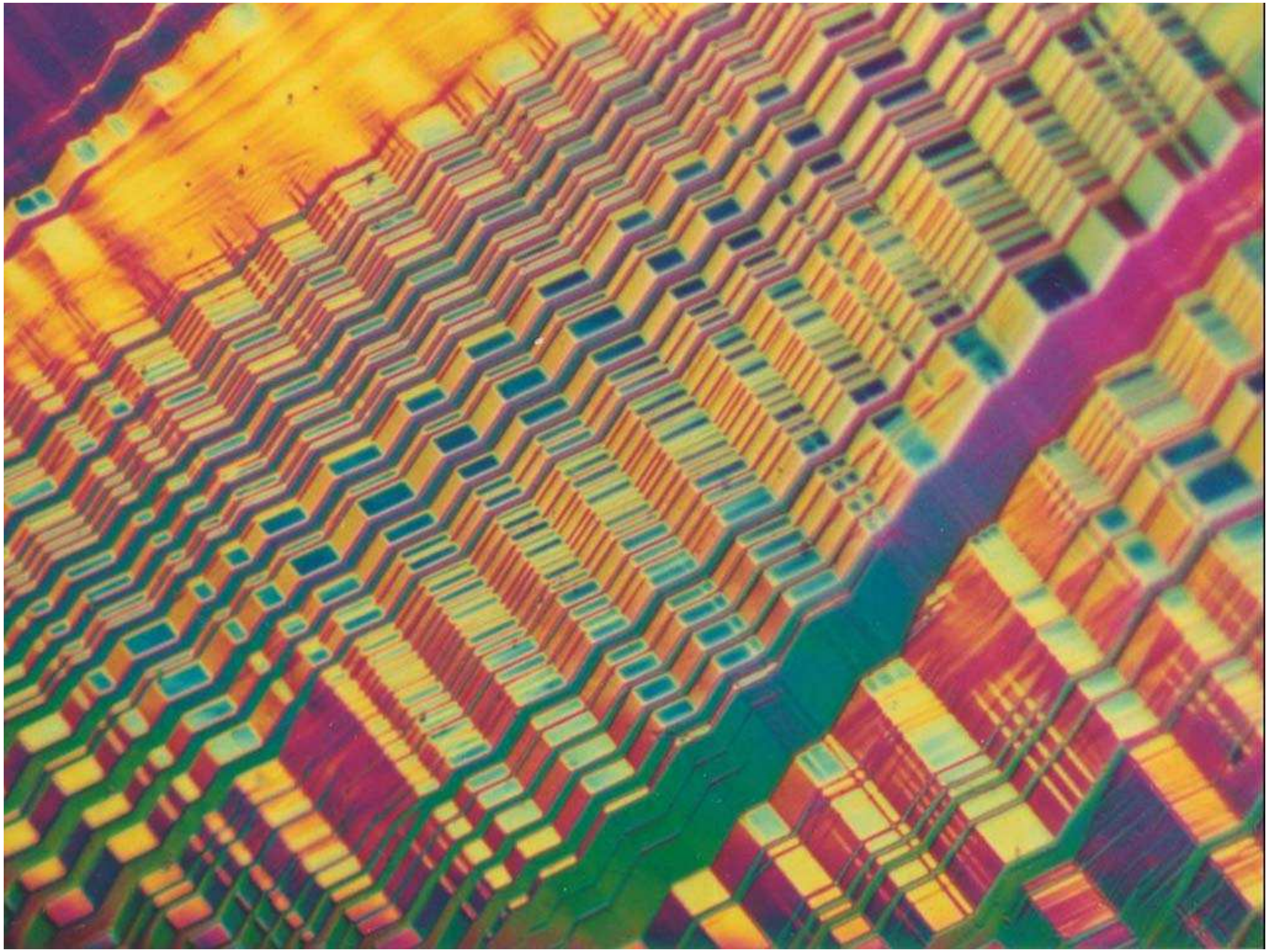
Thin-section photomicrograph of a concrete.

Microstructure



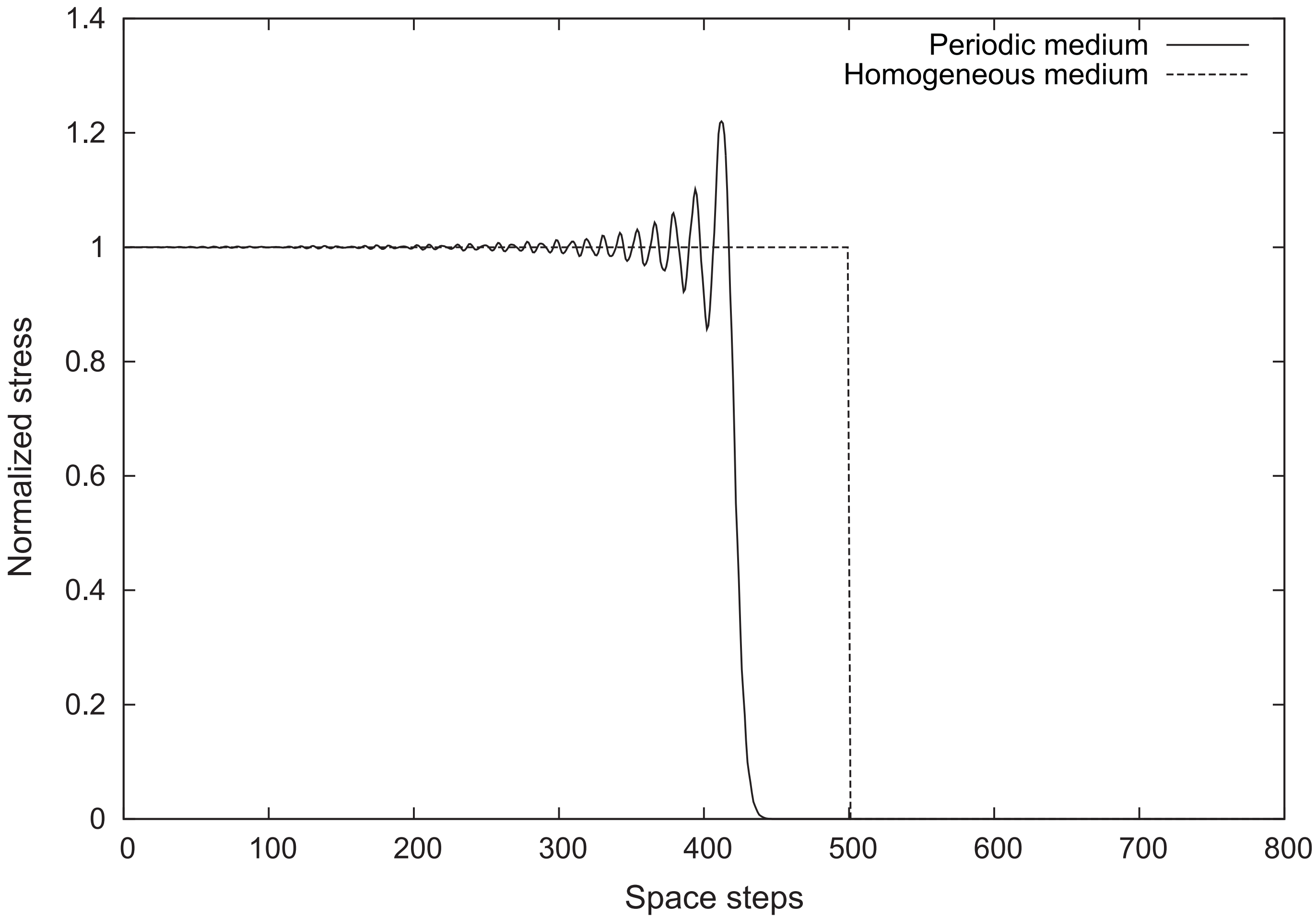
The microstructure of the roller ball, which is made of cast iron. The flakes of graphite are surrounded by ferrite, the brown is the pearlite

Microstructure



Shape memory allow Cu-Al-Ni.

Example of microstructure behavior



Response of two different media on a step-wise loading.

Microstructure model

Wave equation

- One-dimensional wave equation

$$u_{tt} = c^2(x)u_{xx}$$

u is the displacement, c is the elastic wave speed, which is constant for homogeneous medium, but changing at alternating layers in periodic medium.

Generalized wave equations

- Linear version of the Boussinesq equation for elastic crystals (cf. Maugin, 1995)

$$u_{tt} = c^2 u_{xx} + c^2 l^2 A_{22} u_{xxxx}$$

  where l is an internal length parameter and A_{22} is dimensionless coefficient

- The Love-Rayleigh equation for rods accounting for lateral inertia (cf. Love, 1944)

$$u_{tt} = c^2 u_{xx} + l^2 A_{21} u_{xxtt}$$

  This equation is derived also by Maugin (1999); Wang and Sun (2002); Fish et al (2002)

Generalized wave equations

- The more general model combining the two dispersion models (Engelbrecht and Pastrone, 2003)

$$u_{tt} = \left(c^2 - c_A^2\right)\ u_{xx} + l^2 A_2 \left(u_{tt} - c^2 A_1\ u_{xx}\right)_{xx}$$

- The Maxwell-Rayleigh model of anomalous dispersion (cf. Maugin, 1995)

$$u_{tt} = c^2\ u_{xx} + \frac{l^2 A_0}{c^2}\left(u_{tt} - c^2\ u_{xx}\right)_{tt}$$

Generalized wave equations

- The ”causal” model for the dispersive wave propagation (Metrikine, 2006)

$$u_{tt} = c^2 u_{xx} + l^2 A_{21} u_{xxtt} + c^2 l^2 A_{22} u_{xxxx} - \frac{l^2}{c^2} A_{23} u_{tttt}$$

- The most general one-dimensional model (Engelbrecht, Berezovski, Pastrone and Braun, 2005)

$$u_{tt} = \left(c^2 - c_A^2\right) \; u_{xx} - p^2 \left(u_{tt} - c^2 \; u_{xx}\right)_{tt} + \\ + p^2 \; c_1^2 \left(u_{tt} - c^2 \; u_{xx}\right)_{xx}$$

where p is dimensionless coefficient

Dual internal variables approach

Free energy

- The simplest free energy dependence is a quadratic function (Engelbrecht et al., 2005)

$$\overline{W} = \frac{\rho_0 c^2}{2} u_x^2 + A\alpha u_x + \frac{1}{2} B\alpha^2 + \frac{1}{2} C\alpha_x^2 + \frac{1}{2} D\beta^2$$

where ρ_0 is the matter density, A,B,C and D are material parameters, α and β are internal variables.

- Stress components

$$\sigma = \frac{\partial \overline{W}}{\partial u_x} = \rho_0 c^2 u_x + A\alpha, \quad \eta = -\frac{\partial \overline{W}}{\partial \alpha_x} = -C\alpha_x$$

A nondissipative case

- Interactive internal force

$$\tau = -\frac{\partial \overline{W}}{\partial \alpha} = -Au_x - B\alpha$$

- Evolution equations in nondissipative case

$$\alpha_t = -RD\beta, \quad \beta_t = -R(\tau - \eta_x)$$

where R is a coefficient

(Van, Berezovski, Engelbrecht, 2008)

- Evolution equation for the primary internal variable

$$\alpha_{tt} = R^2 D(\tau - \eta_x)$$

A nondissipative case

- Equations of motion in terms of stresses

$$\rho_0 u_{tt} = \sigma_x$$

$$I\alpha_{tt} = -\eta_x + \tau$$

where $I = 1/(R^2 D)$.

It is worth to note that the same equations are derives in (Engelbrecht, Cermelli and Pastrone, 1999) based on different considerations.

A nondissipative case

- Equations of motion

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + A\alpha_x$$

$$I\alpha_{tt} = C\alpha_{xx} - Au_x - B\alpha$$

- First space derivative of the primary internal variable

$$\alpha_x = -\frac{I}{B}\alpha_{ttx} + \frac{C}{B}\alpha_{xxx} - \frac{A}{B}u_{xx}$$

- Third derivatives

$$\frac{A}{\rho_0}\alpha_{xxx} = \left(u_{tt} - c^2 u_{xx}\right)_{xx}, \quad \frac{A}{\rho_0}\alpha_{ttx} = \left(u_{tt} - c^2 u_{xx}\right)_{tt}$$

Generalized wave equation

- Generalized wave equation

$$u_{tt} = c^2 u_{xx} + \frac{C}{B}\left(u_{tt} - c^2 u_{xx}\right)_{xx} - \frac{I}{B}\left(u_{tt} - c^2 u_{xx}\right)_{tt} - \frac{A^2}{\rho_0 B} u_{xx}$$

- Most general model (Engelbrecht, Berezovski, Pastrone and Braun, 2005)

$$u_{tt} = \left(c^2 - c_A^2\right) u_{xx} - p^2 \left(u_{tt} - c^2 u_{xx}\right)_{tt} + \\ + p^2 c_1^2 \left(u_{tt} - c^2 u_{xx}\right)_{xx}$$

- Identification:

$$A^2 = c_A^2 B \rho_0, \quad C = I c_1^2, \quad B = I/p^2$$

Numerical simulations

Equations of motion

- Equations of motion

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + A\alpha_x$$

$$I\alpha_{tt} = C\alpha_{xx} - Au_x - B\alpha$$

- Introducing microvelocity ω as follows:

$$\omega_x := -RD\beta$$

Conservation laws

- Macromotion

Balance of linear momentum

$$\rho_0 v_t = \rho_0 c^2 \varepsilon_x + A \alpha_x$$

Kinematic compatibility

$$\varepsilon_t = v_x$$

- Microstructure evolution

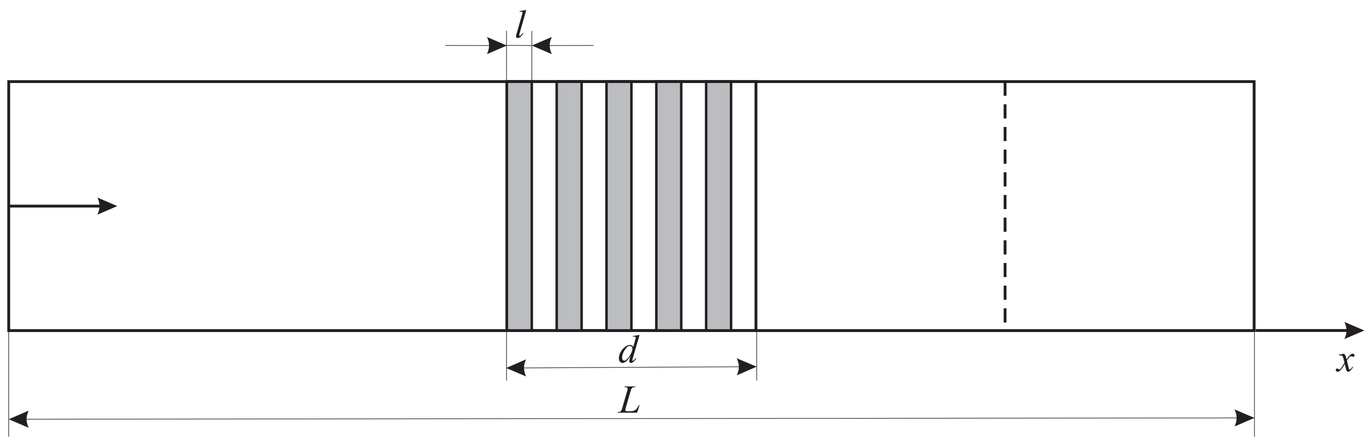
$$I w_t = C \alpha_x - \int (A\varepsilon + B\alpha) dx$$

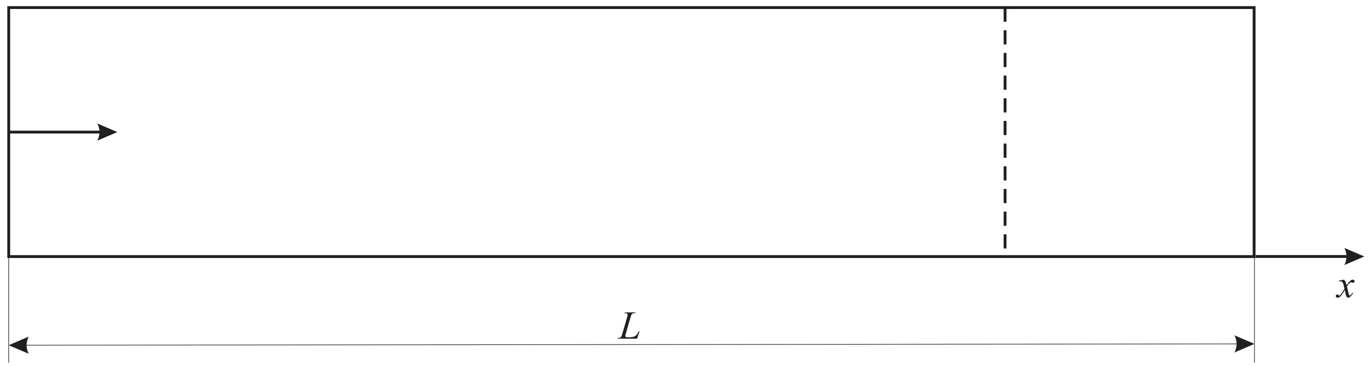
Kinematic compatibility at micro-level

$$\alpha_t = w_x$$

Numerical simulations

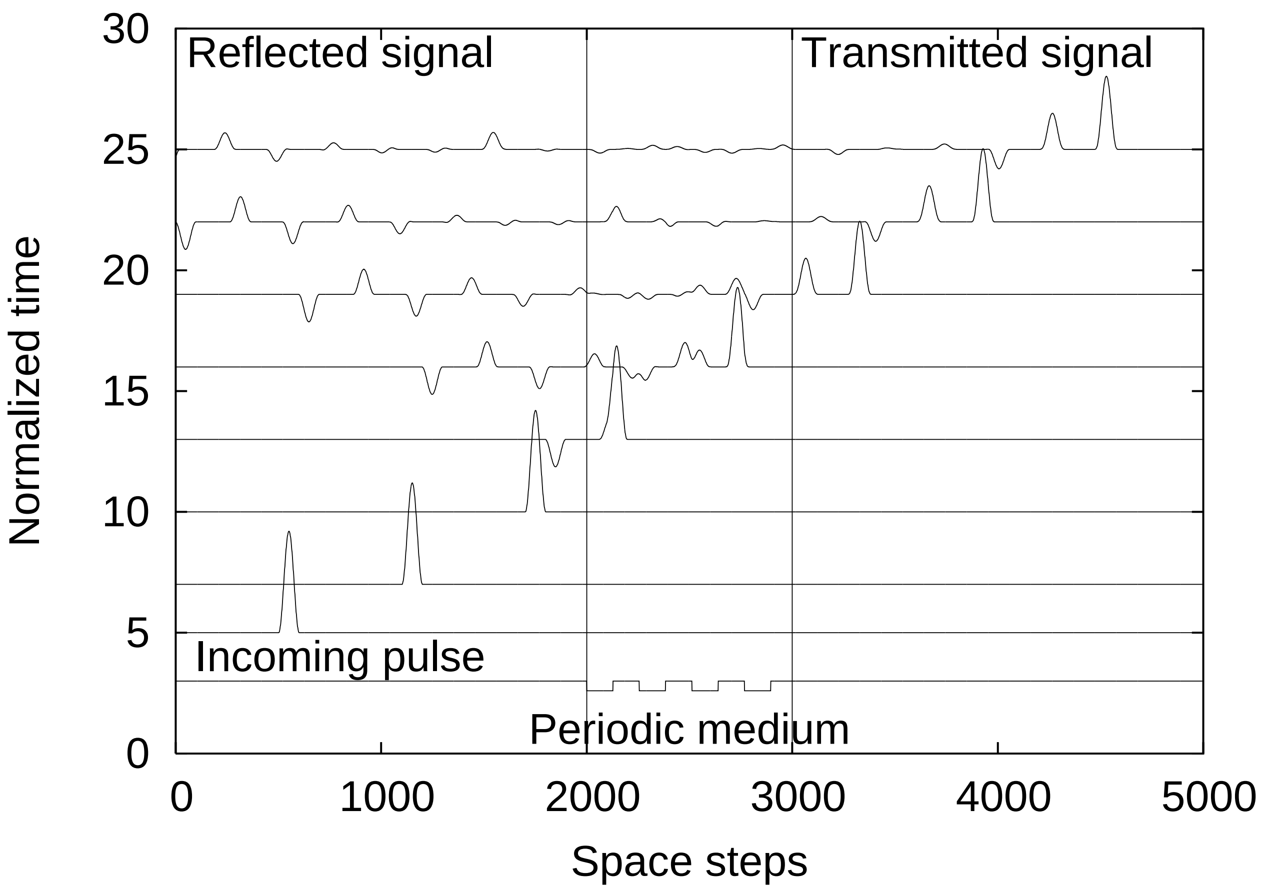
- Geometry of a test problem





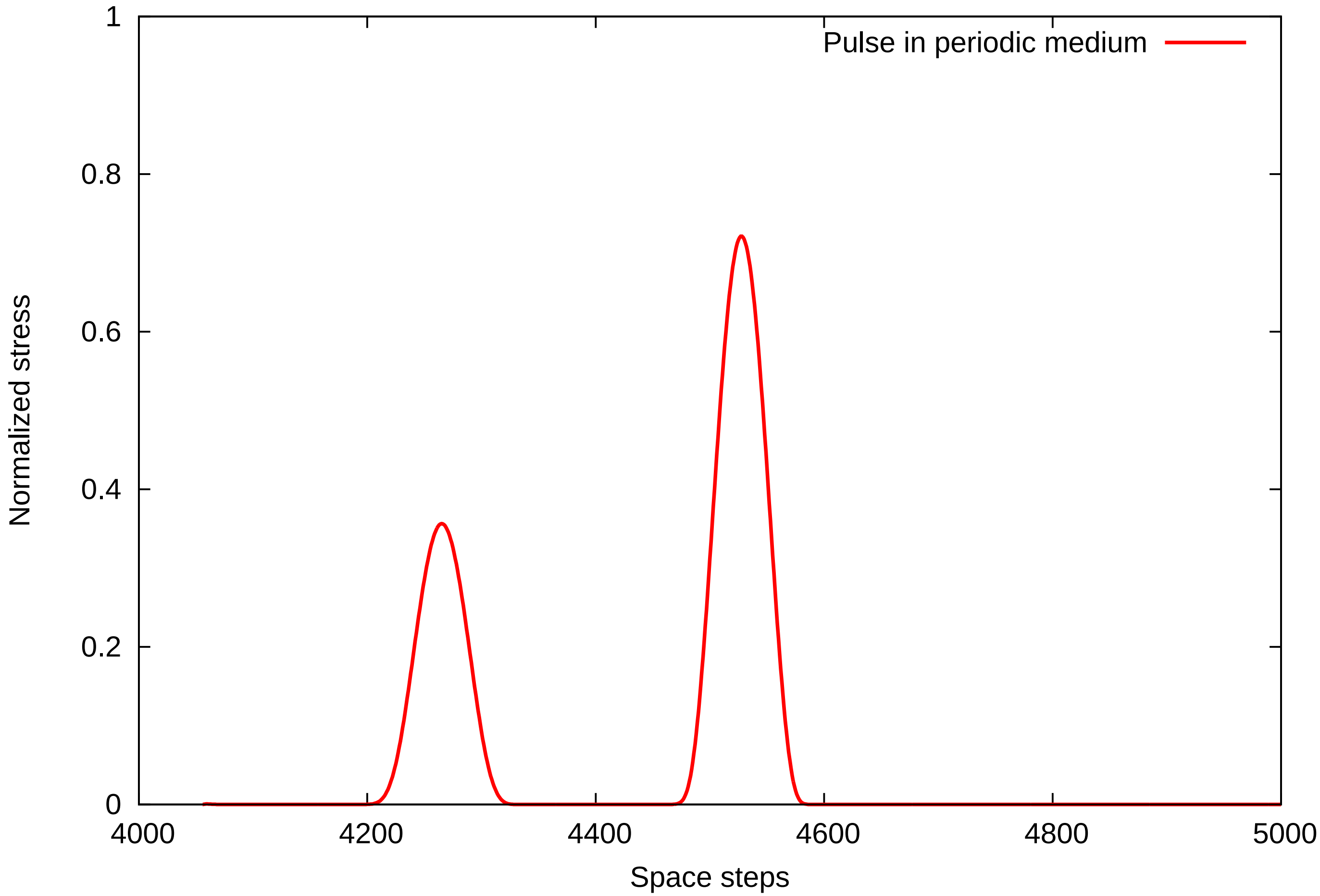
Numerical simulations

- Scattering of a pulse by a periodic multilayer



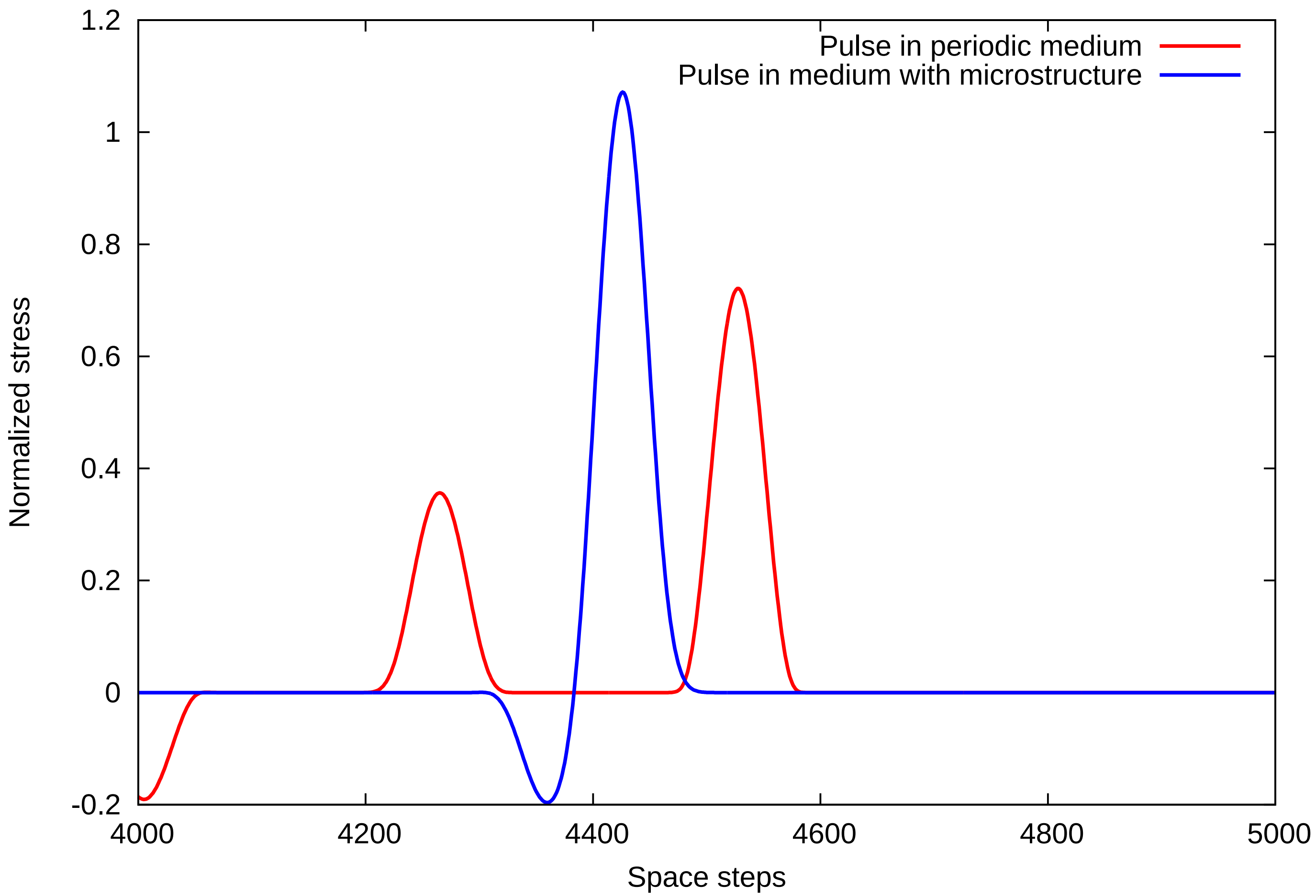
Numerical simulations

- More close look



Numerical simulations

- Microstructure modelling ($l = 128$ space steps, $d = 1000$ space steps)



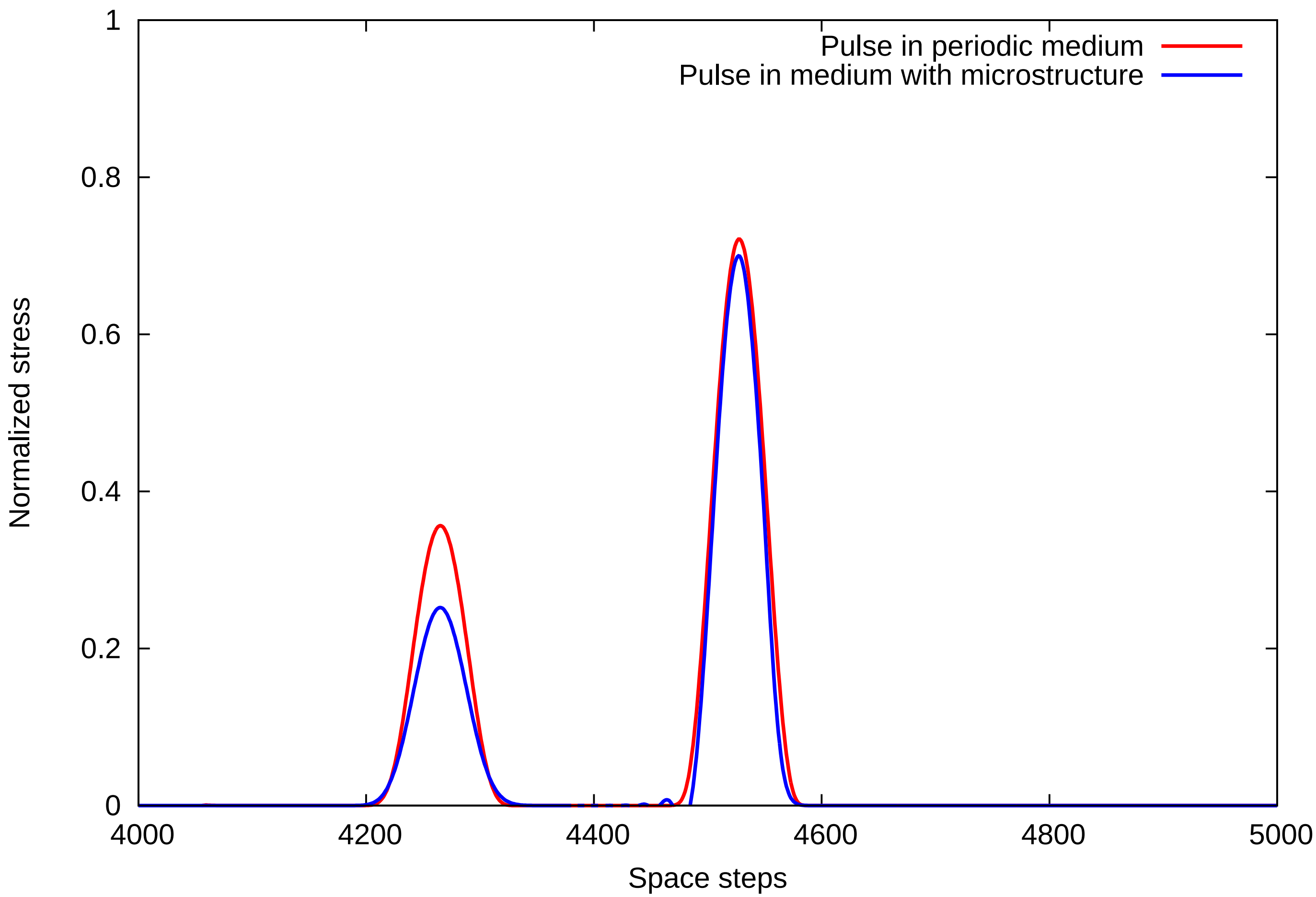
Modification of microstructure model

- Changing sign of interactive internal force

$$I w_t = C \alpha_x + \int (A\varepsilon + B\alpha)\, dx$$

Numerical simulations

- Result with modified model ($l = 128$ space steps, $d = 1000$ space steps)



Numerical simulations

- ❖ Outline
- Motivation
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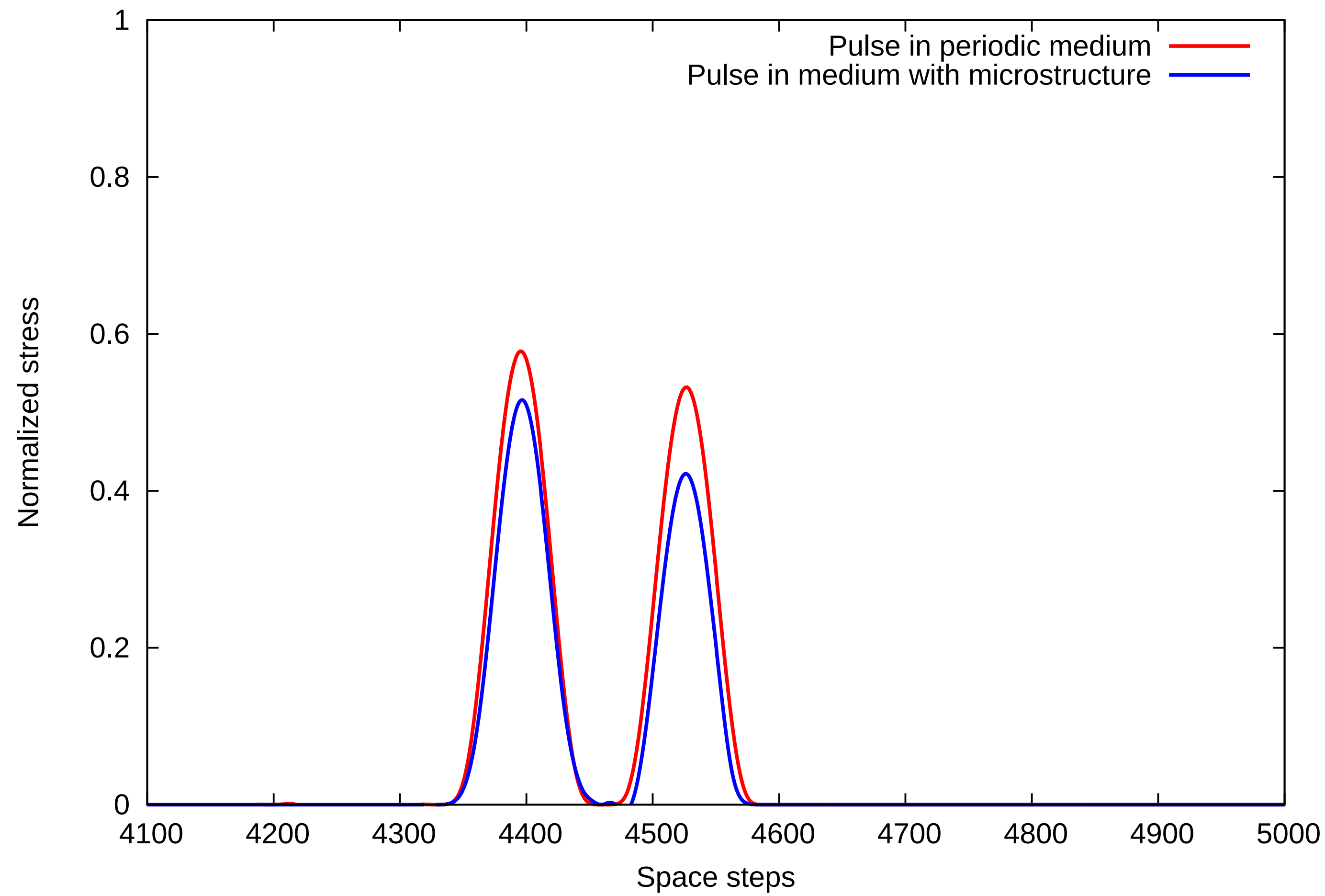
- ❖ Conservation laws
- ❖ Numerical simulations
- ❖ Modification of microstructure model
- ❖ Cubic nonlinearity
- ❖ Conclusions

- Microstructure modelling ($l = 64$ space steps, $d = 1000$ space steps)



Cubic nonlinearity

- Free energy function

$$\overline{W} = \overline{W}_{quadratic} + \overline{W}_{cubic}$$

$$\overline{W}_{cubic} = \frac{1}{6} N u_x^3 + \frac{1}{6} M \alpha_x^3$$

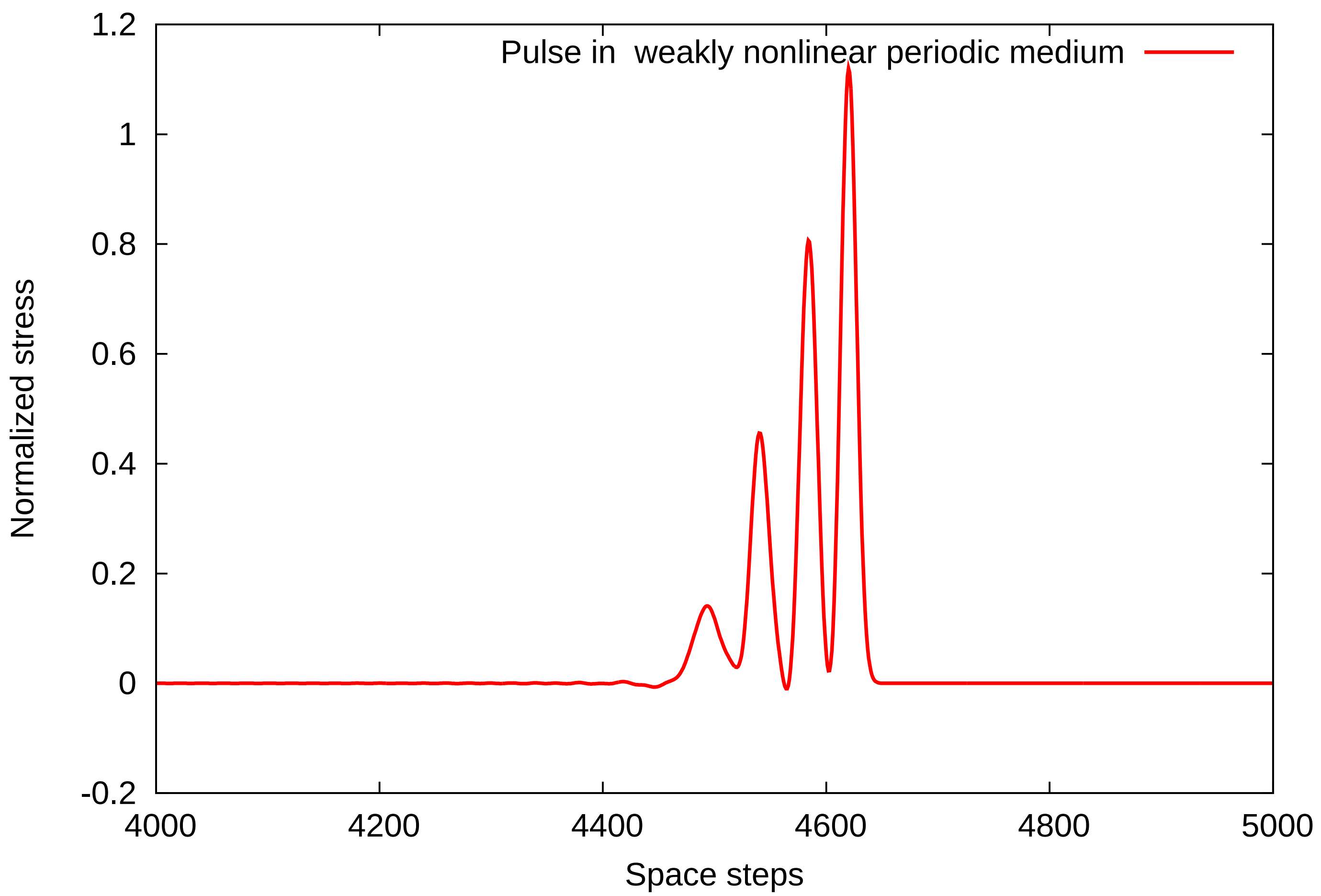
- Equations of motion

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + N u_x u_{xx} + A \alpha_x$$

$$I \alpha_{tt} = C \alpha_{xx} + M \alpha_x \alpha_{xx} + A u_x + B \alpha$$

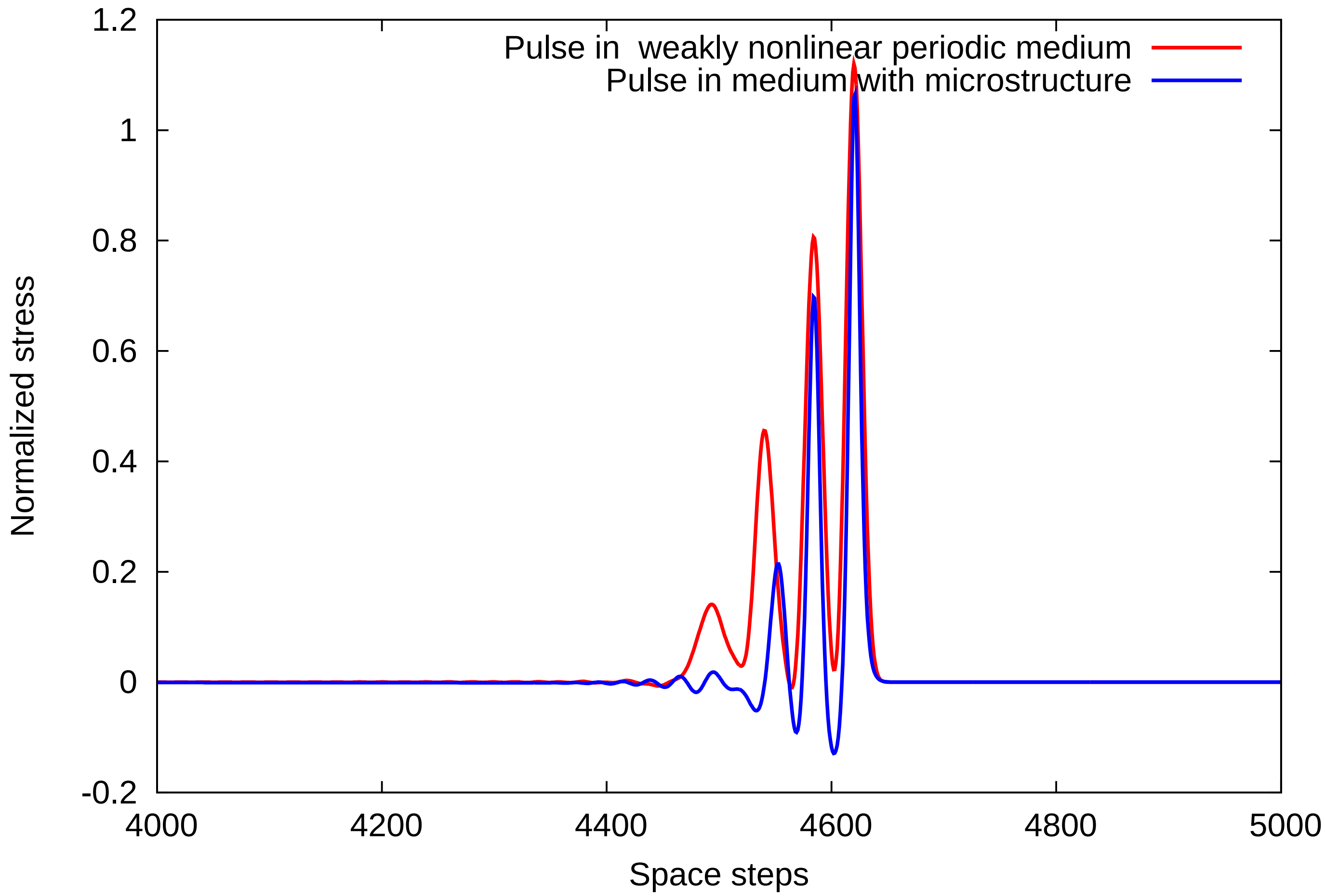
Numerical simulations

- Pulse in periodic nonlinear media ($l = 4$ space steps, $d = 2000$ space steps)



Numerical simulations

- Pulse in periodic nonlinear media ($l = 4$ space steps, $d = 2000$ space steps)



Conclusions

- Numerical simulations were performed to validate microstructure model
- It is shown that some improvements of model should be made to obtain consistency with direct calculation
- Further improvements are needed