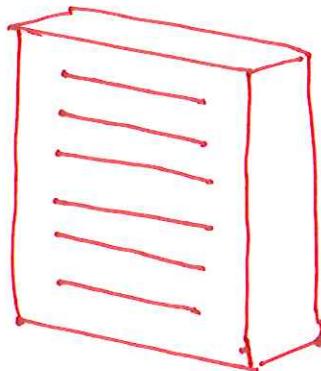


# 3<sup>rd</sup> Moscow Workshop on Biomathematics

Institute  
of  
Numerical  
Mathematics  
R A S



The hybrid discrete-continuous models: asymptotic  
and numerical study

P. Kurbatova, G. Panasenko, V. Volpert

Institute Camille Jordan  
UMR CNRS 5208  
University of Lyon

— october 2011 —

# OUTLINE

- - Motivation
- - DDA linear version
  - existence / uniqueness
  - homogenization
- - DDA with a feed-back (non-linear setting)
  - existence
  - homogenization
- - Possibility of a partial homogenization
- Conclusion

$$\frac{\partial c}{\partial t} = \mathcal{D} \Delta c - nc + nG(p)$$

cell motion

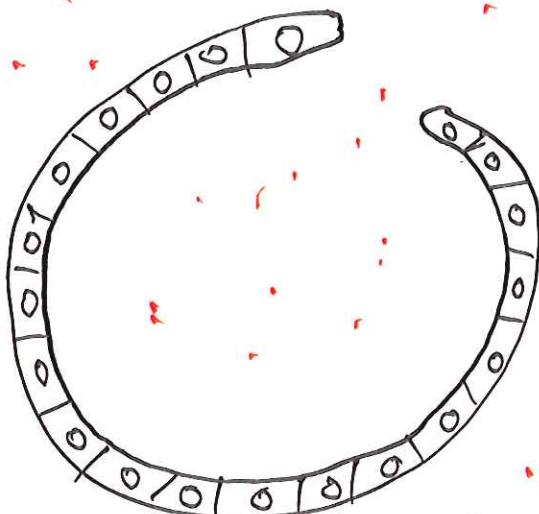
$$x + \mu x + H(\nabla n, c) = 0$$

diffusion - absorption

$$\frac{dp}{dt} = F(p, c)$$

extra-cellular  
matrix

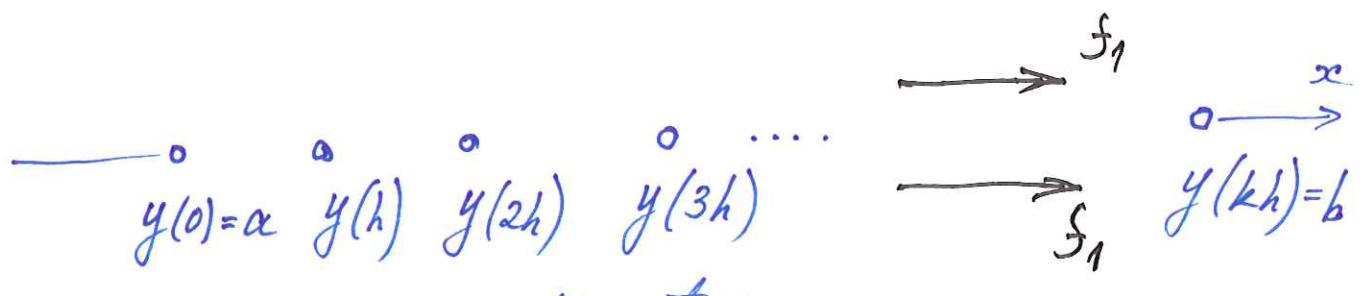
Anabaena



# Motivation



initial position



new coordinates  
under the force  $f_1$

$$\begin{cases} y''(x) = f_1(x), x \in (0, 1) \\ y(0) = a, \quad y(1) = b \end{cases} \quad (1)$$

$$-R < a < b < R,$$

$f_1 \in C([0, 1])$  such that

$y$  increases .

# Diffusion-Discrete Absorption

$$\left\{ \begin{array}{l} u''(x) - h \sum_{j=0}^k \alpha \delta(x - y(jh)) u(x) = f_2(x), \\ x \in (-R, R) \end{array} \right.$$

$$u'(-R) = 0, \quad u(R) = 0 \quad (2)$$

$$\begin{aligned} & - \left( \int_{-R}^R u'(x) \varphi'(x) dx + \sum_{j=1}^k \alpha h u(y(jh)) \varphi(y(jh)) \right) \\ &= \int_{-R}^R f_2(x) \varphi(x) dx \end{aligned} \quad (3)$$

$$+ \varphi \in H_{0R}^1 = \{ \varphi \in H^1(-R, R) \mid \varphi(R) = 0 \}.$$

Theorem 1.1. Let  $\alpha, h > 0$ ,  $kh = 1$ ,  
 $f_2 \in L^2 \Rightarrow \exists! \text{ sol. of (3)}$

# Homogenization (continualisation)

$$\left\{ \begin{array}{l} \bar{u}''(x) - \alpha \bar{u}(x) (y^{-1}(x))' \chi_{[a,b]}^{(x)} = \\ = f_2(x), \quad x \in (-R, R) \\ \bar{u}'(-R) = 0, \quad \bar{u}(R) = 0 \end{array} \right. \quad (4)$$

where  $y$  is a monotone  
solution of (1),  $f_2 \in C$ ,  
 $\chi_{[a,b]}$  is the charact. func.

Theorem 2.1.

$$\| u - \bar{u} \|_{H^1} = O(h).$$

$$\|\kappa - \bar{\kappa}\|_{H^1} \leq \sqrt{2R^2 + 1} \sqrt{2R} M h,$$

$$M = \alpha \left( \left( 4\alpha R^{\frac{5}{2}} \frac{1}{K_0} \|f_2\|_{L^2} + \right. \right. \\ \left. \left. + \|f_2\|_{L^1} \right) (|b-a| + 2\|f_1\|_{L^1}) + \right. \\ \left. + 2R^{\frac{3}{2}} \|f_2\|_{L^2} \right)$$

$$K_0 = \min_{[0,1]} \int_0^x f_1(\theta) d\theta + (b-a) -$$

$$- \int_0^1 \int_0^t f_1(\theta) d\theta dt > 0$$

(y →).

# DDA with a feed-back

$$u''(x) = \alpha h \sum_{j=0}^K \delta(x - Y_j^{(u)}) u(x) + f(x),$$

$$x \in (-R, R),$$

$$u'(-R) = 0, u(R) = 0,$$

$$Y_j^{(u)} = jh E_0 \left( 1 + q F[u] \right)^{-1},$$

$$j = 0, \dots, K,$$

$$F[u] = \int_0^{E_0} u(x) dx.$$

$$f \in C, \alpha > 0, h > 0, Kh = 1;$$

$$0 < E_0 < R/2, q > 0.$$

Theorem 3.1  $\exists \alpha_*, q_* > 0$ ,

indep. of  $h$ , such that if

$0 < \alpha < \alpha_*$ ,  $0 < q < q_*$  then

$\exists$  a solution.

Proof :

Schauder fixed point

$$Tu = u$$

theorem for

$$T : C([-R, R]) \rightarrow C([-R, R])$$

$$(Tv)(x) = - \int_{-R}^R \left\{ \lambda v(t) + \int_{-R}^t f_2(\theta) d\theta \right\} dt$$

$$(\lambda v)(x) = h \lambda \sum_{j: Y_j^v \leq x} v(Y_j^v)$$

# Homogenization (continualisation)

$$\bar{u}''(x) = \alpha \quad \left( \frac{1+qF[u]}{E_0} \chi_{[0, Y_K^u]}(x) \bar{u}(x) + f(x), \quad x \in (-R, R), \quad \bar{u}'(-R) = 0, \quad \bar{u}(R) = 0 \right)$$

$(y^{-1})' = \text{const}$

$$+ f(x), \quad x \in (-R, R),$$

$$\bar{u}'(-R) = 0, \quad \bar{u}(R) = 0$$

Theorem 4.1.  $\exists \alpha_*, q_* > 0,$

such that if  $0 < \alpha < \alpha_*$ ,  $0 < q < q_*$  indep. of  $h$

$$0 < \alpha < \alpha_*, \quad 0 < q < q_*$$

then  $\exists!$  solution in a ball.

Theorem 4.2. For

$$0 < \alpha < \alpha^*, \quad 0 < q < q^*,$$

$$\| u - \bar{u} \|_C = O(h)$$

## Partial homogenization

$$\bar{u}''(x) - \alpha \bar{u}(x) \left( y^{-1}(x) \right)' \gamma_{[a,b]}(x) = \\ = f_2(x), \quad x \in (-R, R) \setminus [c, d]$$

$$\bar{u}''(x) - h \sum_{j: y(jh) \in [c, d]} \alpha \delta(x - y(jh)) \bar{u}(x) \\ = f_2(x), \quad x \in \underline{\underline{[c, d]}}$$

$$[\bar{u}] = 0, \quad [\bar{u}'] = 0 \quad \text{in } c, d,$$

$$\bar{u}'(-R) = 0, \quad \bar{u}(R) = 0$$

It is a hybrid model

Theorem 5.1.  $\exists!$  sol.

$$- \left( \int_{-R}^R \bar{u}'(x) \varphi'(x) dx + \right.$$

$$+ \int_{[a,b] \setminus [c,d]} \alpha \bar{u}(x) \varphi(x) (y^{-1}(x))' dx +$$

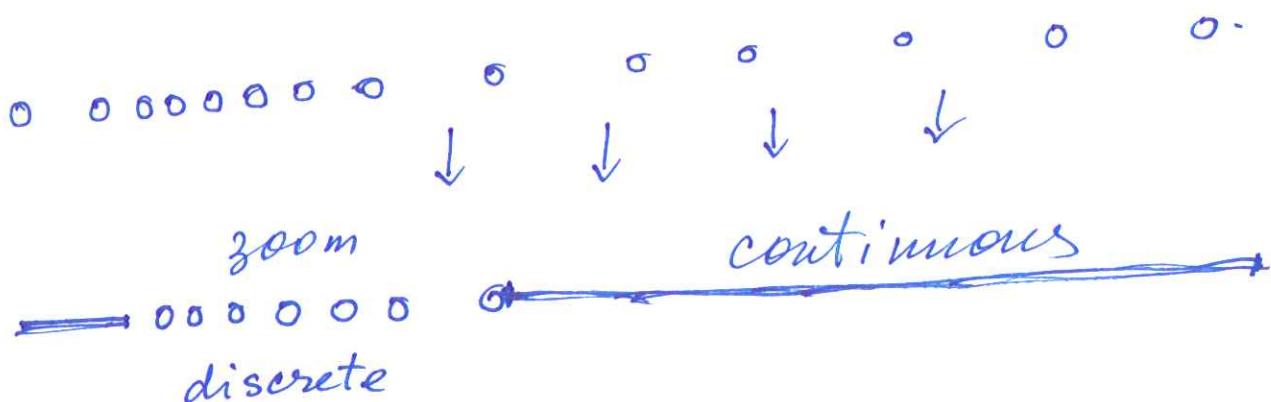
$[a,b] \setminus [c,d]$

$$+ \sum_{j: y(jh) \in [c,d]} \alpha h \bar{u}(y(jh)) \varphi(y(jh)) =$$

$$= \int_{-R}^R f_2(x) \varphi(x) dx$$

$\forall \varphi \in H_{\text{OR}}^1$

Theorem 5.2.  $\|u - \bar{u}\|_{H^1} = O(h)$ .



## Conclusion

Passage micro → macro  
in discrete models DDA

Possibility of combined  
hybrid description with  
the discrete zoom.

## References

- [1] N.S. Bakhvalov, Averaging of partial differential equations with rapidly oscillating coefficients, *Doklady Acad. Nauk SSSR* 224 (2), pp. 351–355, 1975.
- [2] N.S. Bakhvalov, *Méthodes Numériques*. Edition Mir, Moscow, 1973.
- [3] N. Bessonov, V. Volpert, Dynamic models of plant growth- Mathematics and Mathematical Modelling. Publibook, 2006.
- [4] X. Blanc, C. Le Bris, P.L. Lions, From molecular models to continuum mechanics. *Archive for Rational Mechanics and Analysis*, 164, 4, pp. 341-381, 2002.
- [5] X. Blanc, C. Le Bris, F. Legoll, Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics, *ESAIM: M2AN*, Vol. 39, n. 4, 797–826, 2005.
- [6] M. Born, K. Huang, *Dynamical Theory of Crystal Lattices*, Oxford U. P., London, 1954.
- [7] D. Caillerie, A. Muorad, A. Raoult, Discrete homogenization in graphene sheet modeling. *Journal of Elasticity*, vol. 84, pp. 33–68, 2006.
- [8] M. Betoue Etoughe, G. Panasenko, Partial homogenization of discrete models, *Applicable Analysis*, vol. 87, n. 12, pp. 1425–1442, 2008.
- [9] S.M. Kozlov, Averaging of difference schemes, *Math. USSR Sb.*, Vol 57, pp. 351–369, 1987.
- [10] I.A. Kunin, *Media with Microstructure*, I. Vol. 26, Spring-Verlag, Berlin, New-York, 1982; II. Vol. 44, Spring-Verlag, Berlin, New-York, 1983.
- [11] R. Orive, E. Zuazua, Finite difference approximation of homogenization problems for elliptic equations, *Multi-scale Methodes and Simulation* 4, 2005, pp. 36–87.
- [12] G. Panasenko, *Multi-scale Modeling for Structures and Composites*, Springer, 2005.
- [13] G. Panasenko, Partial homogenization: continuous and discrete versions, *Math. Models and Methods in Applied Sciences*, 17, 8, 2007, pp. 1183–1209.
- [14] A. Piatnitski, E. Rémy, Homogenization of elliptic difference operators, *SIAM J. Math. Anal.*, 33,1, pp. 53–83, 2001.
- [15] V. Shenoy, R. Miller, E.B. Tadmor, D. Rodney, R. Philips, M. Ortiz, An adaptive finite element approach to atomistic-scale mechanics - The Quasi-Continuum Method, *J. Mech. Phys. Solids* 47, p. 611, 1999.

## **GRANTS**

**SFR MOMAD of the University of Saint Etienne and  
ENISE ( the Ministry of the  
Research and Education of France),**

**the joint French-Russian PICS CNRS grant  
"Mathematical modeling of blood diseases"**

**the grant no. 14.740.11.0875 "Multiscale problems:  
analysis and methods" of the Ministry of Education and  
Research of Russian Federation.**