High Performance Computing and Grid in Latvia: Status and Perspectives

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BaltGrid, 2004, Vilnius, Lithuania

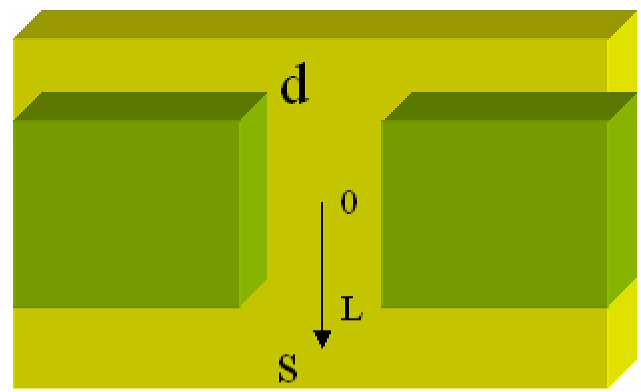
Introduction

- What?
  - HPC actual problems
    - · charge and mass transfer in a non-linear media
    - · ferroelectric/ferromagnetic and critical indices
- Why?
  - Multidimensional and complicated geometry problems need to be supported by effective calculations
- How?
  - Numerical methods, Monte Carlo simulations
  - Parallel programming
- So what?
  - Grid connections to supercomputers

Charge transfer : IMCS University of Latvia (Latvia) & MCI Southern Denmark University, supported by CIRIUS (Denmark)

Optically sensitive semiconductor plasma

$$\frac{\partial n_\alpha}{\partial t} - \frac{\partial J_n^\alpha}{\partial x} = -\left(R^\alpha - G^\alpha\right) \quad , \quad \alpha = c, \quad \alpha = e$$



$$\frac{3}{2}\frac{\partial}{\partial t}\left(n_\alpha T_n^\alpha\right) + \frac{\partial}{\partial x} S_n^\alpha = -J_n^\alpha \frac{\partial \varphi}{\partial x} + P_n^\alpha$$

$$\frac{\partial p_\alpha}{\partial t} + \frac{\partial J_p^\alpha}{\partial x} = -\left(R^\alpha - G^\alpha\right)$$

$$\frac{3}{2}\frac{\partial}{\partial t}\left(p_\alpha T_p^\alpha\right) + \frac{\partial}{\partial x} S_p^\alpha = -J_p^\alpha \frac{\partial \varphi}{\partial x} + P_p^\alpha \quad , \quad J_p^\alpha = -\mu_n^\alpha p_\alpha \frac{\partial \varphi}{\partial x} - \frac{\partial}{\partial x}\left(\mu_p^\alpha p_\alpha T_p^\alpha\right)$$

$$\frac{\partial}{\partial x}\left(\kappa \frac{\partial \varphi}{\partial x}\right) = n_c - p_c + n_e - p_e - \left(N_d - N_a\right) \; , S_n^\alpha = -C_e^\alpha \left(-\mu_n^\alpha n_\alpha \frac{\partial \varphi}{\partial x} T_n^\alpha + \tfrac{\partial}{\partial x}\left(\mu_n^\alpha n_\alpha \left(T_n^\alpha\right)^2\right)\right)$$

$$J_n^\alpha = -\mu_n^\alpha n_\alpha \frac{\partial \varphi}{\partial x} + \frac{\partial}{\partial x}\left(\mu_n^\alpha n_\alpha T_n^\alpha\right) \quad , \quad S_p^\alpha = -C_h^\alpha \left(\mu_p^\alpha p_\alpha \frac{\partial \varphi}{\partial x} T_p^\alpha + \tfrac{\partial}{\partial x}\left(\mu_p^\alpha p_\alpha \left(T_p^\alpha\right)^2\right)\right)$$

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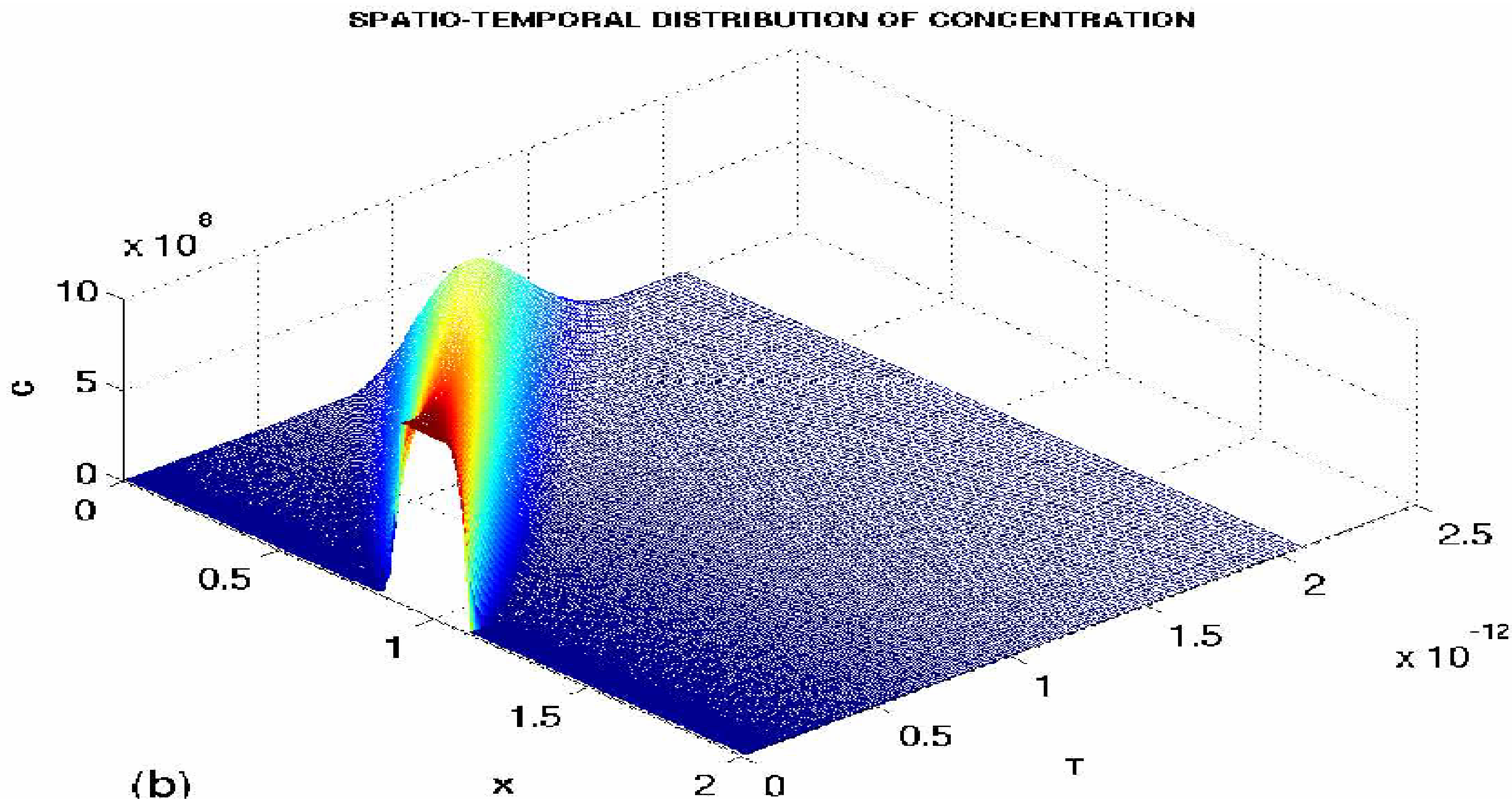


R.V.N. Melnik and J. Rimshans, Monotone schemes for time-dependentenergy balance models, ANZIAM J. 45 (E), C729-C743, 2004 (Proc. of 11thComputational Techniques and Applications Conference, CTAC-2003)

R.V.N. Melnik and J.Rimshans, Numerical Analysis of Fast Transport in Optically Sensitive Semiconductors, Special Issue of DCDIS – 2003, DCDIS Series B, ISSN 1492-8760, Guelph, Ontario, Canada, p.1-6.

Shock waves: IMCS University of Latvia (Latvia) & DMR National Science Foundation (USA)

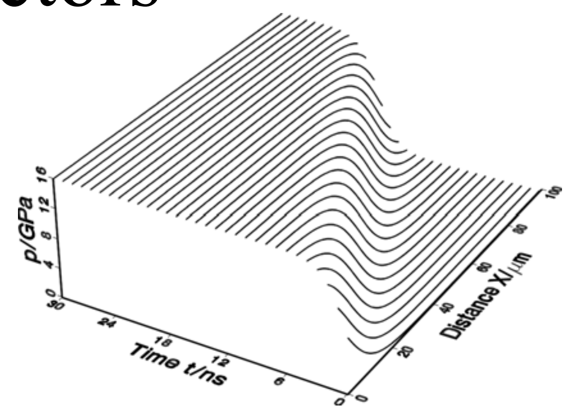
Shocked solid conductors

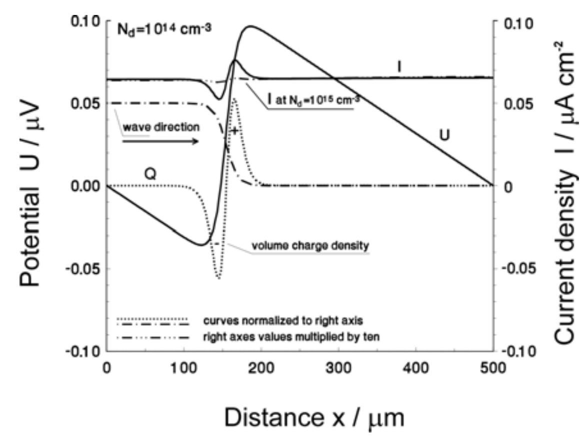
$$\nabla \mathbf{J}_n = -\frac{\partial n}{\partial t}$$

$$\mathbf{J}_n = -D_n\left(\nabla n - \frac{q}{k_B T} n \nabla(\varphi + \varphi_T)\right)$$

$$\nabla(\varepsilon \nabla \varphi) = -\frac{q}{\varepsilon_0}(N_d - n)$$

$$q \nabla \varphi_T = -m \frac{\partial v}{\partial t}$$





B.Martuzans. Yu. Skryl, M.M. Kuklja, *Dynamic Response of the Electrone-Hole System in the shocked silicon.* Latvian Journal of Physics and Technical Sciences. N4, pp. 56-68, 2003

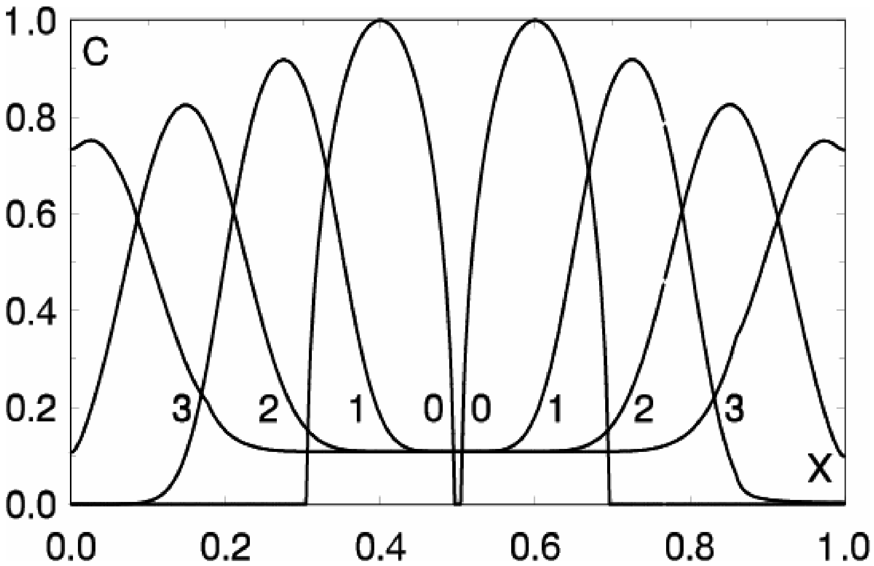
Yu. Skryl, M.M.Kuklja, Numerical simulation of electron and hole diffusion in shocked silicon, AIP Conference Proceedings, 706(1), 267-270 (2004).

Convection-diffusion : IMCS University of Latvia (Latvia) & SMS&EPCC University of Edinburgh, supported by Royal Society (UK)

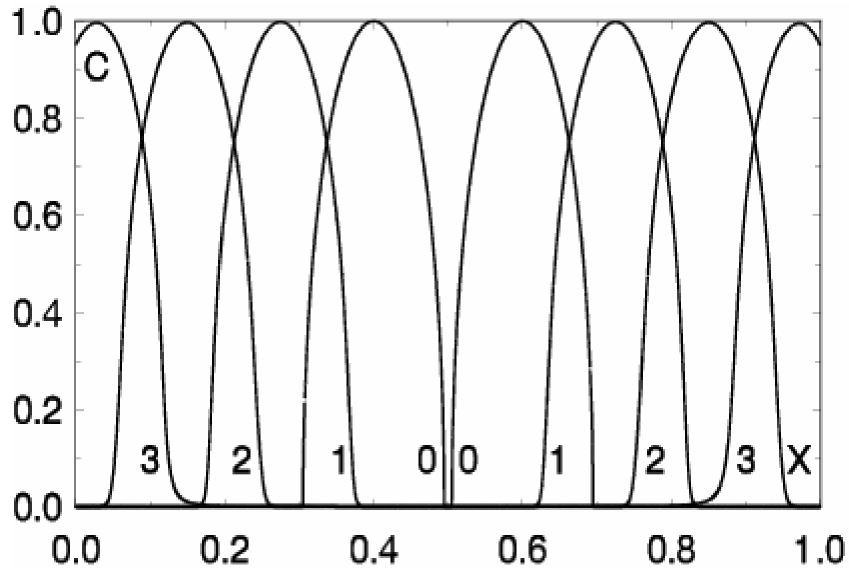
Advective transport

$$\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial x} = \frac{\partial}{\partial x} K \frac{\partial C}{\partial x}$$

$\frac{K}{v} = 10^{-2}$



$\frac{K}{v} = 0$



J.Rimshans and N.Smyth, Monotone exponential difference scheme for advection diffusion equation, Submitted for Numerical methods for partial differential equations, 2004.

Ferroelectric materials under alternate driving:

ISSP&IMCS University of Latvia (Latvia)

Probability density: key entities

Probability density of polarization

Variation of energy

Thermal noise strength is the most delicate counterpart of theory. Understanding of its dynamical origin is in progress

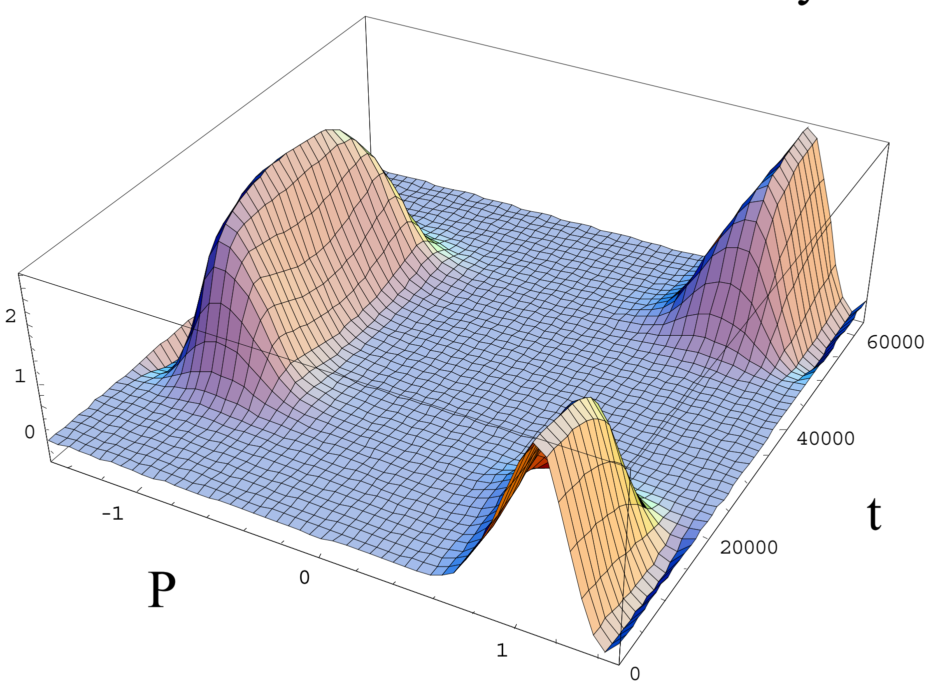
$$\dot{\rho}(P,t) = \frac{\partial}{\partial P}\left[\frac{\delta H}{\delta P(x)}\rho(P,t)\right] + \Theta\frac{\partial^2 \rho(P,t)}{\partial P^2}$$

J. Hlinka and E. Klotins, Application of elastostatic Green function tensor technique to electrostriction in cubic, Hexagonal and Orthorombic crystals, J. Phys.: Condens. Matter 15 (2003) 5755-5764

Ferroelectric materials under alternate driving:

ISSP&IMCS University of Latvia (Latvia)

Probability density of polarization



Parameters of the model:

Quartic Landau-Ginzburg energy functional+periodic driving.
Amplitude of driving voltage = A0/2
Dimensionless frequency = 10^(-4)
Diffusion constant (noise strength = 1/20
Polarization = first moment of the instantaneous probability density

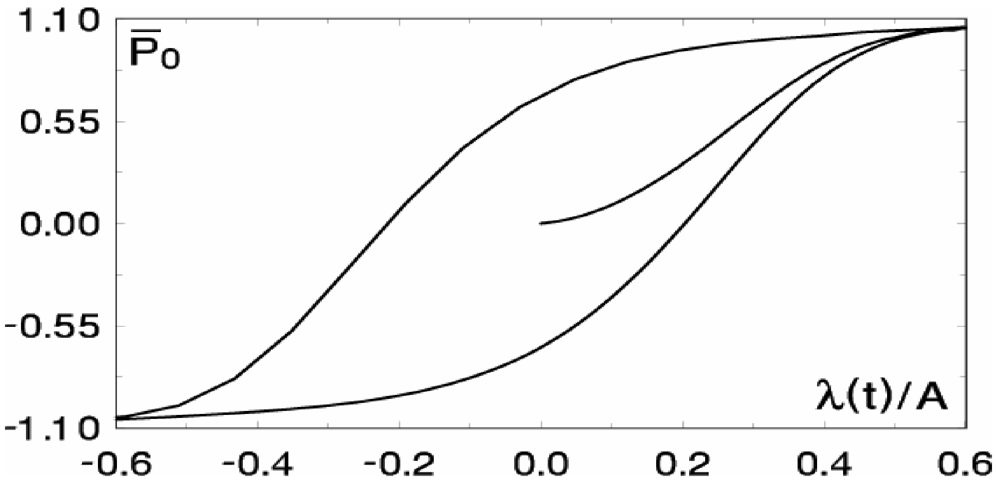
E. Klotins, Relaxation dynamics of metastable systems: application to polar medium, Physica A, 340 (2004) 196-200

Ferroelectric materials under alternate driving:

IMCS University of Latvia (Latvia)

Spatially homogeneous case

$$\frac{1}{\gamma}\frac{\partial f}{\partial t} = \frac{\partial}{\partial P_0}\left\{ Vf\left[\alpha P_0 + \beta P_0^3 - A\sin(\omega t)\right] + \theta \frac{\partial f}{\partial P_0}\right\}$$



$$\gamma = V = \beta = 1$$
$$\alpha = -1$$
$$\theta = 0.05$$
$$A = 0.309$$
$$\omega = 10^{-3}$$

J. Kaupužs, J. Rimshans, Polarization kinetics in ferroelectrics with regard to fluctuations, Cond-mat/0405124, 2004.

Critical exponents: IMCS University of Latvia (Latvia)

φ^4 perturbation theory

$$H/T = \int dx \left(r\,\varphi^2(x) + c(\nabla\varphi(x))^2 + u\,\varphi^4(x) \right)$$

$$\frac{1}{2G_i(k)} = r_0 + ck^2 - \frac{\partial D(G)}{\partial G_i(k)}$$ Dyson equation

Predicted for 3D Ising model:

Susceptibility exponent $\gamma = 5/4$

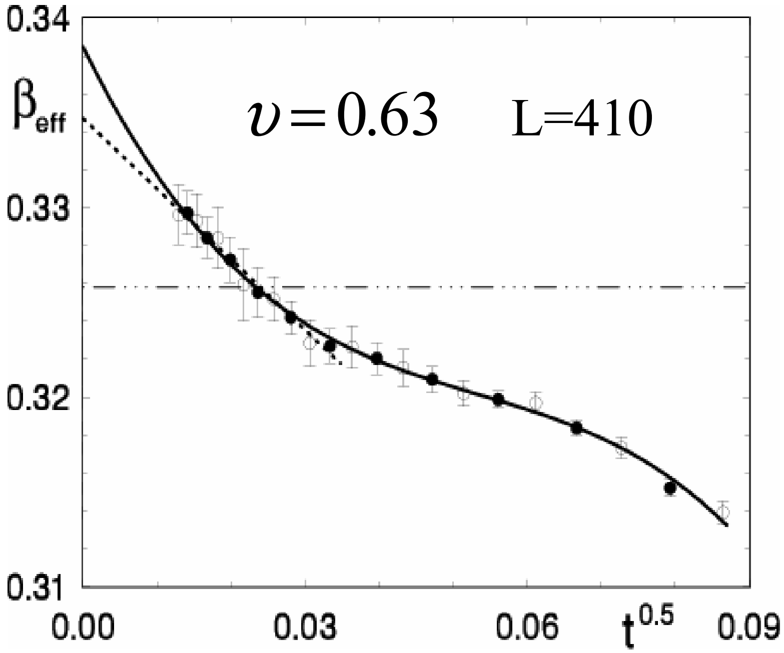
Correlation length exponent $\upsilon = 2/3$

Magnetization exponent $2\beta = d\upsilon - \gamma$

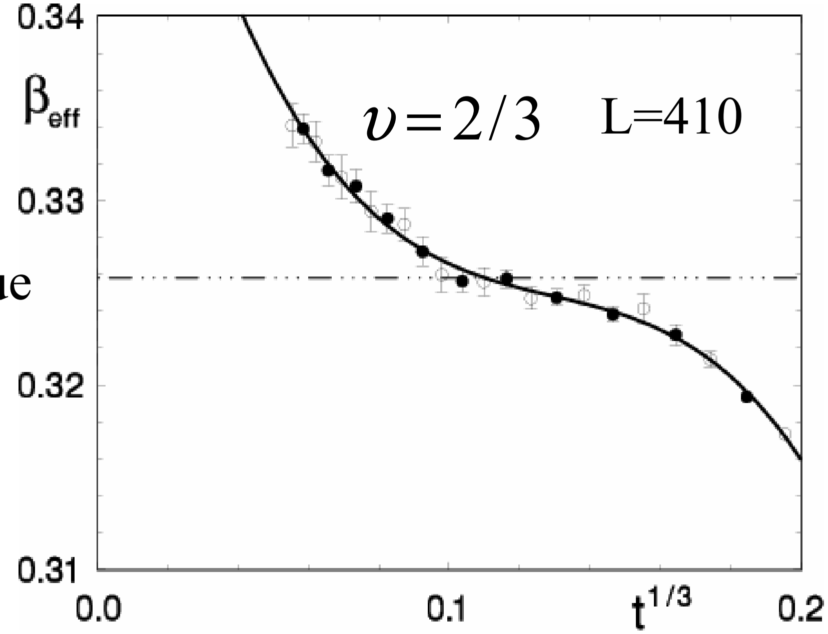
J.Kaupužs, Ann. Phys. (Leipzig) 10 (2001) 4, 299-331

Critical exponents: IMCS University of Latvia (Latvia)

Monte Carlo simulation results: magnetization exponent



RG value



$$L = 256\,(t_0 / t)^{\upsilon}$$

J.Kaupužs, Proceedings of SPIE, vol. 5471, pp. 480-491, 2004; e-print cond-mat/0405197

Main problems

- Convection – diffusion
  - Advective transport
  - Convection
- Monte Carlo simulations
- Data transmission
- Training

Advective transport

Ornstein-Uhlenbeck process

$$\frac{\partial C}{\partial t} + (\mu x)\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial x^2}$$

Usual schemes

FTCS, Upwind, LaxWendrof

Monotone condition

$$2s \le 1, \quad s = K\tau / h^2,$$

$$\tau \le \frac{1}{2}\frac{h^2}{K}$$

Unconditionally monotone scheme

$$\left(\Lambda(\beta)C^{l+1}\right)_i = \frac{1}{h_i} A_i C_{i-1}^{l+1} + \frac{1}{h_i} B_i C_{i+1}^{l+1} - Q_i C_i^{l+1} = -\frac{C_i^l}{\tau}$$

$$Q_i = \frac{1}{h_i^*}\left(A_{i+1} + B_{i-1}\right) + \frac{1}{\tau}$$

$$A_i = K_{i-1/2}\beta_{i-1/2}\frac{\exp\left(\beta_{i-1/2}\right)}{h_i\left(\left(\exp\left(\beta_{i-1/2}\right)\right) - 1\right)}$$

$$B_i = K_{i+1/2}\beta_{i+1/2}\frac{1}{h_i\left(\left(\exp\left(\beta_{i+1/2}\right)\right) - 1\right)}$$

Advective transport

Ornstein-Uhlenbeck process

TABLE I. Effectiveness of the difference schemes for the case of a uniform grid.

N	$Scheme^a$	$X_L(m/s^{1/2})$	Pc	C_r^*	ϵ	e
	FT			$1.6{\cdot}10^{-12}$	0.015	0.08
	Up			$1.6{\cdot}10^{-12}$	0.015	0.08
1	LW	10^{-4}	$3.4{\cdot}10^{-12}$	$1.6{\cdot}10^{-12}$	0.015	0.08
	CN			$1.8{\cdot}10^{-10}$	0.016	1.9
	ad			$1.8{\cdot}10^{-10}$	0.014	1
	FT			$1.4{\cdot}10^{-4}$		0.08
	Up			$1.4{\cdot}10^{-4}$		0.08
2	LW	1	$3.1{\cdot}10^{-4}$	$1.4{\cdot}10^{-4}$	0.014	0.08
	CN			0.016		1.9
	ad			0.017		1

[a] FT-FTCS,Up-Upwind,LW-Lax-Wendroff,CN-Crank-Nicolson,ad-elaborated scheme.

J.Rimshans and N.Smyth, Monotone exponential difference scheme for advection diffusion equation, Submitted for Numerical methods for partial differential equations, 2004.

Advective transport

Ornstein-Uhlenbeck process

TABLE II. Effectiveness of the difference schemes for the case of a non-uniform grid.

N	*Scheme*	$X_L(m/s^{1/2})$	Pc	C_r^*	ϵ	e
1	CN	10^{-4}	$5.0{\cdot}10^{-13}$	$1.1{\cdot}10^{-9}$	0.015	$2.9{\cdot}10^{-3}$
	ad			$1.3{\cdot}10^{-9}$	0.039	1
2	CN	1	$5.0{\cdot}10^{-5}$	0.087	0.014	$2.9{\cdot}10^{-3}$
	ad			0.1	0.039	1
3	ad	10^{4}	1	10^{4}	0.006	1
4	ad	10^{8}	10^{4}	10^{8}	0.009	1

J.Rimshans and N.Smyth, Monotone exponential difference scheme for advection diffusion equation, Submitted for Numerical methods for partial differential equations, 2004.

Convection-diffusion

Charge transfer

$$\nabla \mathbf{J}_n = -\frac{\partial n}{\partial t}$$

$$\nabla(\varepsilon \nabla \varphi) = -\frac{q}{\varepsilon_0}(N_d - n)$$

$$\mathbf{J}_n = -D_n\left(\nabla n - \frac{q}{k_B T} n \nabla \varphi\right)$$

$$\tau \le \frac{\varepsilon\varepsilon_0}{q}\frac{1}{(\frac{q}{k_B T}D)N_d}$$

Implicit

Half Implicit

Explicit methods

$$\tau \le \frac{1}{2}\frac{h^2}{D}$$

Ferroelectric materials under alternate driving:

IMCS University of Latvia (Latvia)

Fokker-Planck equation

Landau-Ginzburg hamiltonian
$$H = \int dx \left(\frac{\alpha}{2} P^2(x) + \frac{\beta}{4} P^4(x) + \frac{c}{2} (\nabla P(x))^2 - \lambda(x,t) P(x,t) \right)$$

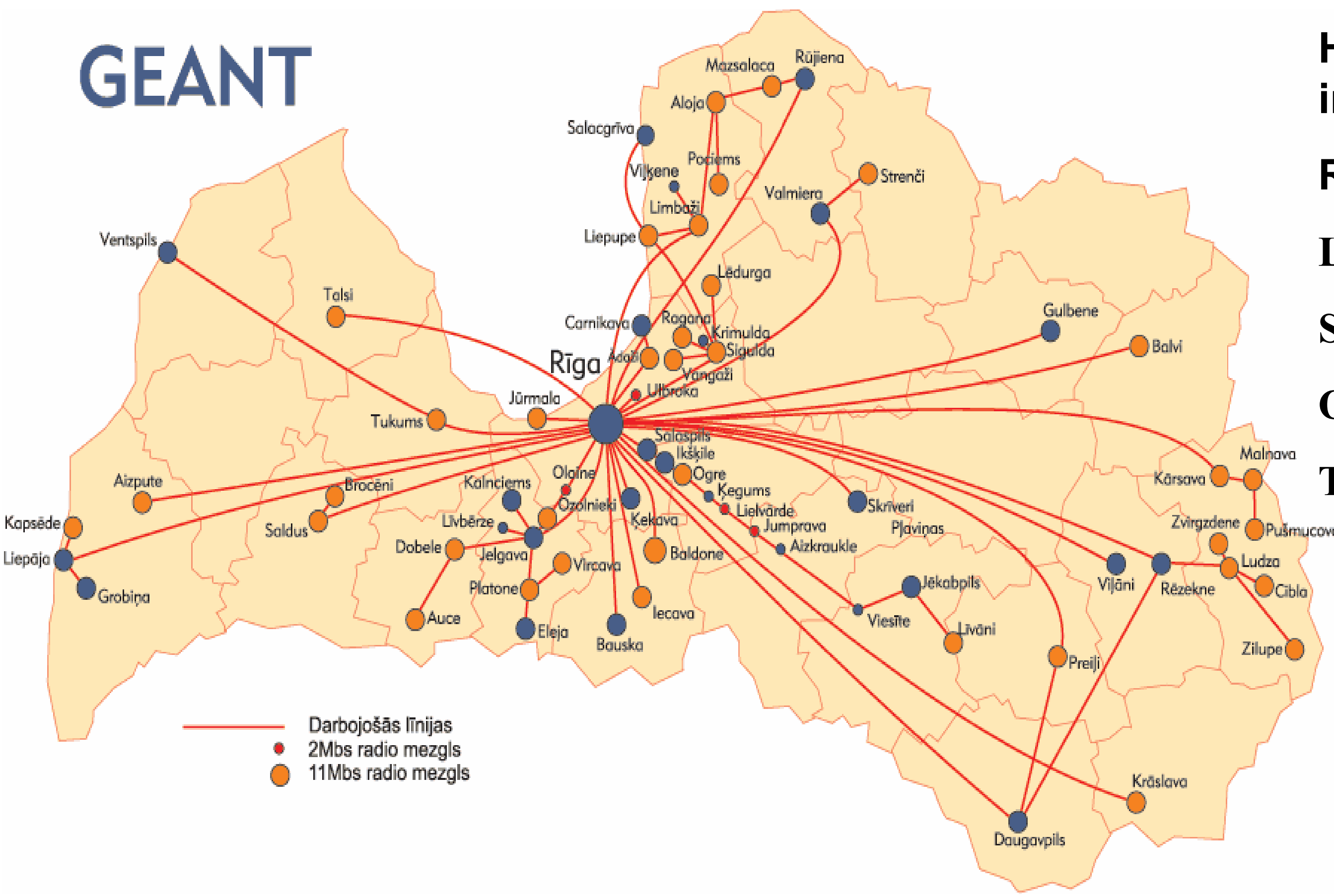
Langevin equation
$$\frac{\partial P}{\partial t} = -\gamma \frac{\partial H}{\partial P} + \xi(x,t)$$

$$\frac{1}{\gamma}\frac{\partial f}{\partial t} = \sum_{n=0}^{2m} \frac{\partial}{\partial P_{k_n}^r} \left\{ \Delta V f \left[\left(\alpha + c k_n^{\ 2} \right) P_{k_n}^r + \beta S_{k_n}^r - \lambda_{k_n}^r(t) \right] + \frac{\theta}{2} \left(1 + \delta_{k_n,0} \right) \frac{\partial f}{\partial P_{k_n}^r} \right\} +$$
$$\sum_{n=1}^{2m} \frac{\partial}{\partial P_{k_n}^i} \left\{ \Delta V f \left[\left(\alpha + c k_n^{\ 2} \right) P_{k_n}^i + \beta S_{k_n}^i - \lambda_{k_n}^i(t) \right] \right\} \quad , \quad 2m+1 \text{ dimensions}$$

J.Kaupužs, J.Rimshans, *Polarization kinetics in ferroelectrics with regard to fluctuations*, cond-mat/0405124, 2004.

GEANT

GEANT – GN2-Multi-Gigabit European Academic Network



Higher education institutions	**47**
Research institutes	**11**
Libraries	**15**
State institutions	**3**
Others	**37**
Total	**113**

Very Long Baseline Interferometry Network