Crystal Growth: Physics, Technology and Modeling

Stanisław Krukowski & Michał Leszczyński
Institute of High Pressure Physics PAS
01-142 Warsaw, Sokołowska 29/37
e-mail: stach@unipress.waw.pl, mike@unipress.waw.pl

Zbigniew Żytkiewicz
Institute of Physics PAS
02-668 Warsaw, Al. Lotników 32/46
E-mail: zytkie@ifpan.edu.pl

Lecture 12. Growth modeling in macoscale

http://www.unipress.waw.pl/~stach/cg-2021-22

Growth modeling – two approaches

- **Modeling in macroscale**
  - transport processes during growth (mass, energy, momentum)
  - strain in nonuniform structures
  - electric properties of electronic structures and devices
  - optical properties of optoelectronic structures and devices
  - crystal morphology

- **Modeling in atomic scale**
  - crystal structure
  - energetic properties
  - kinetic properties
  - optical transitions

Growth modeling - methods

- **Modeling in macroscale**
  - finite difference
  - finite volume
  - finite element

- **Modeling in atomic scale**
  - Monte Carlo
  - molecular dynamics
  - ab initio – density functional theory (DFT)

Conservation laws – compressible fluid

$$\frac{\partial[\rho(\vec{r},t)]}{\partial t} + div\left(\rho(\vec{r},t)\overrightarrow{v}(\vec{r},t)\right) = 0$$

$$\rho(\vec{r},t)\left[\frac{\partial\overrightarrow{v}(\vec{r},t)}{\partial t} + (\vec{v}(\vec{r},t)\cdot\nabla)\overrightarrow{v}(\vec{r},t)\right] = -\nabla p(\vec{r},t) + \mu\Delta\overrightarrow{v}(\vec{r},t) + \rho(\vec{r},t)\overrightarrow{f}(\vec{r},t)$$

$$\frac{\partial\left[C_p(T)T(\vec{r},t)\rho(\vec{r},t)\right]}{\partial t} + \rho(\vec{r},t)C_p(T)(\vec{v}(\vec{r},t)\cdot\nabla)T(\vec{r},t) = div\left(\kappa\nabla T(\vec{r},t)\right) + r_\varepsilon$$

- **6 variables: 3 velocity components, density, pressure, temperature**
- **5 equations of motion + equation of state**

$$p = p(\rho, T)$$

Conservation laws – incompressible fluids

$$div\left(\vec{v}(\vec{r},t)\right) = 0$$

$$\rho_o\left[\frac{\partial\overrightarrow{v}(\vec{r},t)}{\partial t} + (\vec{v}(\vec{r},t)\cdot\nabla)\overrightarrow{v}(\vec{r},t)\right] = \mu\Delta\overrightarrow{v}(\vec{r},t) + \rho_o[\beta_T(T-T_o)+\beta_c c]\overrightarrow{f}(\vec{r},t)$$

$$\rho_o C_p(T)\left[\frac{\partial[T(\vec{r},t)]}{\partial t} + (\vec{v}(\vec{r},t)\cdot\nabla)T(\vec{r},t)\right] = div\left(\kappa\nabla T(\vec{r},t)\right) + r_\varepsilon$$

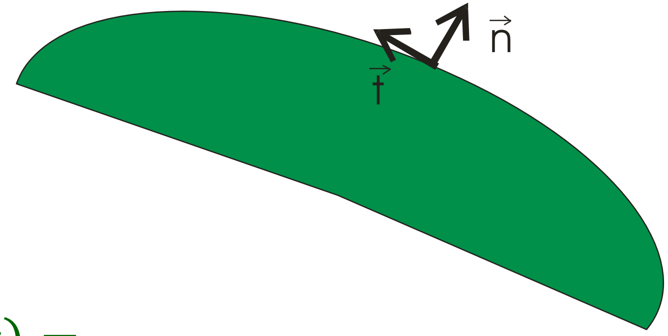
- **5 variables: 3 velocity components, pressure, temperature**
- **5 equations**
- **Additional equation:**

$$\boldsymbol{\rho = \rho_o}$$

Boundary conditions - velocity

- **Solid surfaces – no-slip condition:**

$$\vec{v}(\vec{r},t) = 0$$



- **Solid surface – crystal growth (surface is nonmaterial, no-slip):**

$$\vec{v}(\vec{r},t) \cdot \vec{t}(\vec{r},t) = 0$$

$$\rho_l(\vec{r},t)[\vec{v}(\vec{r},t)c_l(\vec{r},t) - D_l \nabla c_l(\vec{r},t)] \cdot \vec{n}(\vec{r},t) = \rho_s(\vec{r},t)[\vec{u}(\vec{r},t)c_s(\vec{r},t) - D_s \nabla c_s(\vec{r},t)] \cdot \vec{n}(\vec{r},t)$$

$\vec{t}(\vec{r},t)$ **- vector tangential to the surface**

$\vec{n}(\vec{r},t)$ **- vector normal to the surface**

$\vec{u}(\vec{r},t)$ **- crystallization velocity**

Boundary conditions - temperature

- **Solid –vapor/liquid interface – perfect thermal contact:**

$$T_l(\vec{r},t) = T_s(\vec{r},t)$$

- **Solid surface – crystal growth (surface is nonmaterial, no-slip):**

$$[C_l\rho_l(\vec{r},t)\vec{v}_l(\vec{r},t) - C_s\rho_s(\vec{r},t)\vec{v}_s(\vec{r},t)]\cdot\vec{n}(\vec{r},t) =$$
$$[\kappa_l \nabla T_l(\vec{r},t) - \kappa_s \nabla T_s(\vec{r},t) + \rho_s(\vec{r},t)\vec{u}(\vec{r},t)H]\cdot\vec{n}(\vec{r},t) + Q$$

H* – *latent heat

Q* – *radiation flux

Boundary conditions – mathematical categories

- **Dirichlet condition**

$$\boldsymbol{\varphi_l(\vec{r},t) = \varphi_s(\vec{r},t)}$$

- **Neumann condition**

$$\boldsymbol{\nabla\varphi_s(\vec{r},t)\cdot\vec{n}(\vec{r},t) = f_s(\vec{r},t)}$$

- **Mixed condition**

$$\boldsymbol{F[\nabla\varphi_s(\vec{r},t)\cdot\vec{n}(\vec{r},t)] + G[\varphi_s(\vec{r},t)] = f_s(\vec{r},t)}$$

Boundary conditions – physical interpretation

- **Dirichlet boundary condition: temperature, concentration – local equilibrium between phases**

$$T_l(\vec{r},t) = T_s(\vec{r},t) \qquad C_l(\vec{r},t) = kC_s(\vec{r},t)$$

- **Dirichlet boundary condition – tangential component of the velocity disappears**

$$\vec{v}(\vec{r},t) \cdot \vec{t}(\vec{r},t) = 0$$

- **Neumann boundary condition – predetermined flows such as crystallization velocity, dissolution, flux**

$$D\nabla C(\vec{r},t) \cdot \vec{n}(\vec{r},t) = R(\vec{r},t)$$

- **Mixed condition – crystallization velocity in function of the supersaturation**

$$D\nabla C(\vec{r},t) \cdot \vec{n}(\vec{r},t) = k\sigma = k\left(\frac{C - C_{eq}}{C_{eq}}\right)$$

Solution methods – approximation

- **Conservation law: classical field ϕ – mathematical structure**

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial(v_i\rho\phi)}{\partial r_i}=\frac{\partial}{\partial r_j}\left[\Gamma\frac{\partial\phi}{\partial r_j}\right]+q_\phi$$

Approximate algorithm

- **Scalar field is replaced by its representation in the mesh sites - pre-processing**
- **Boundary condition are enforced – pre-processing**
- **Solution - processing**
- **Result – represented by continuous functions - post-processing**

Mesh generation - preprocessing

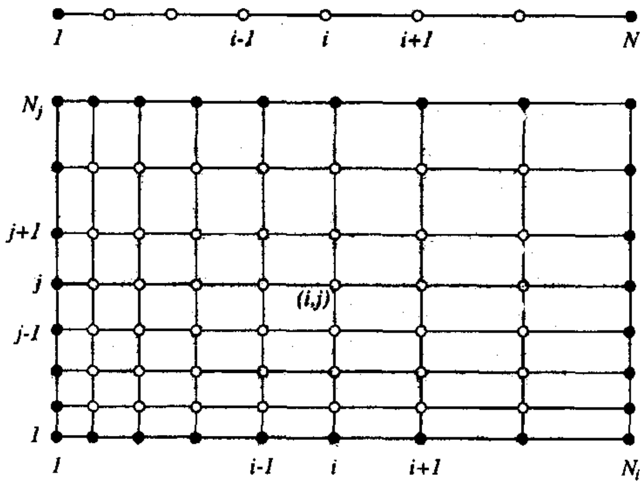
Mesh types:

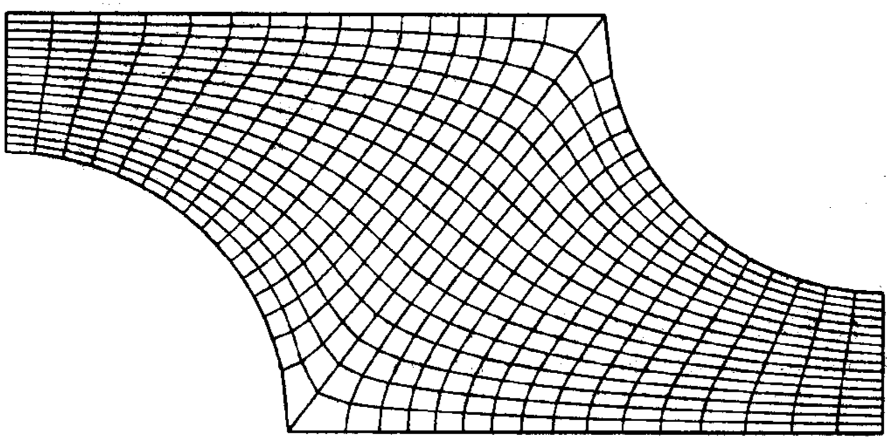
- **Regular (structural)**
- **Block-regular (block-structural)**
- **Complex**
- **Irregular**

Regular mesh (structural)

Regular mesh – coordinate system

- **Lines belonging to the same family do not cross**
- **Lines belonging to different families cross once only**



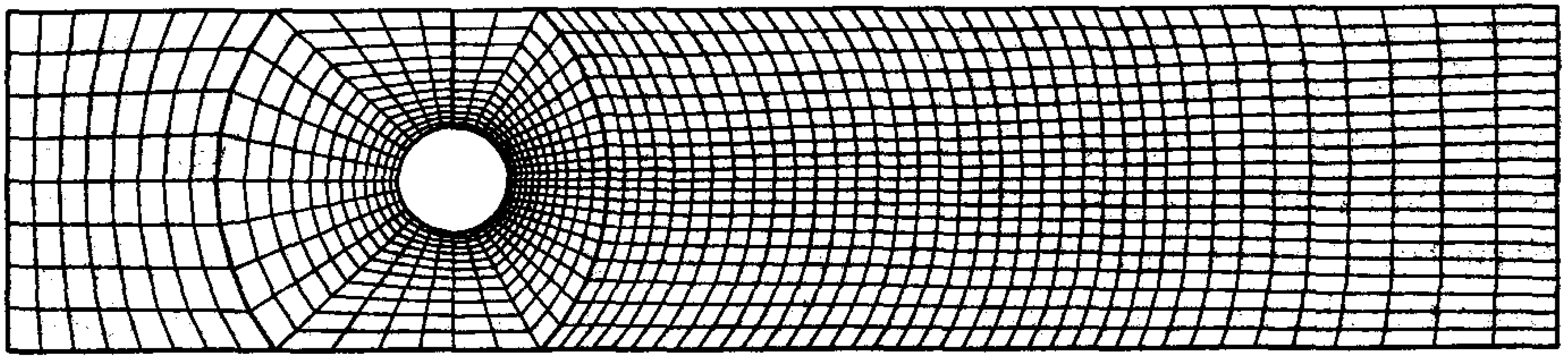


Examples: 1-d and 2-d regular orthogonal mesh

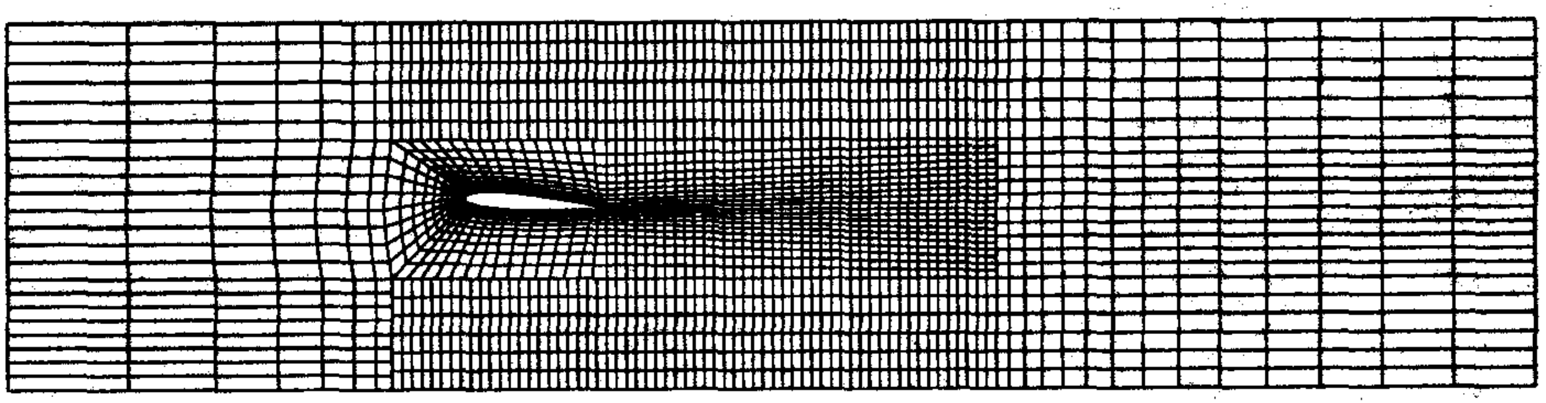
Example: 2-d regular nonorthogonal mesh designed for calculation of the flow between two parallel pipes

Block-regular mesh

- **Segments are regular – the sum is not**



Example: block-regular nonorthogonal mesh. The sites are compatible. .

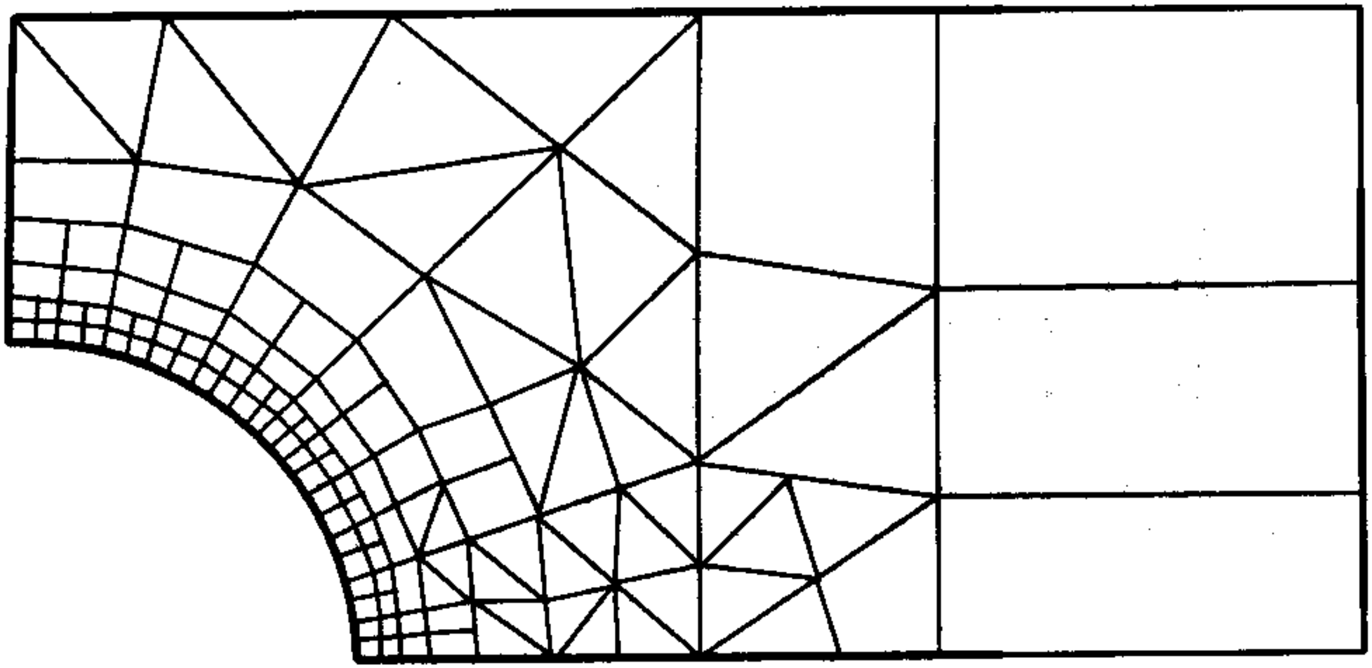


Example: block-regular nonorthogonal mesh. The sites are not compatible.

.

Non-structural mesh

- **Mesh filling any volume (area), e.g. triangular mesh**



Example: 2-d mesh composed of triangular and tetra-angular elements

- **Extension – adaptive mesh**

Solution methods – algorithms

- **Conservation law: classical field ϕ**

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(v_i\rho\phi)}{\partial r_i} = \frac{\partial}{\partial r_j}\left[\Gamma\frac{\partial\phi}{\partial r_j}\right] + q_\phi$$

  - **Finite difference method**
  - **Finite volume method**
  - **Finite element method**

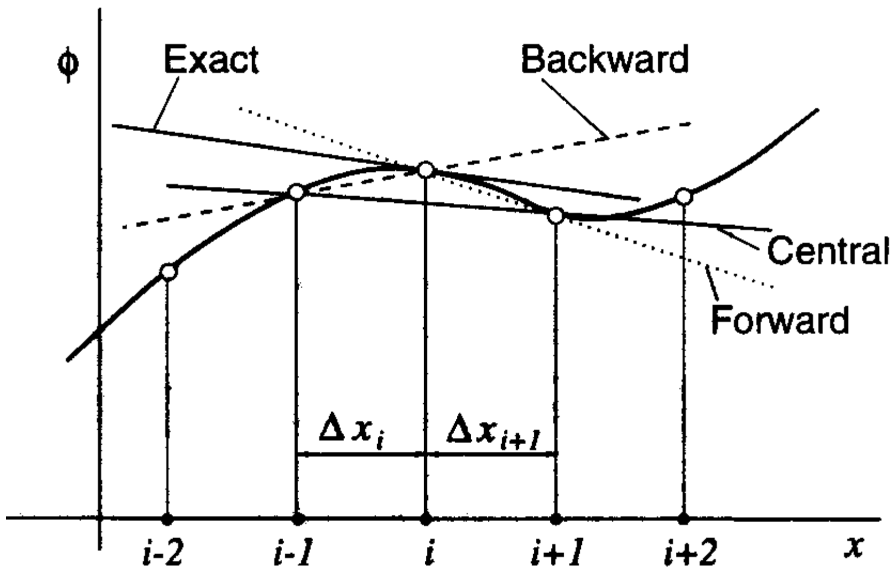
Finite difference method

- **L. Euler (XVIII century) – derivative are replaced by finite difference between sites**

$$\frac{\partial \phi}{\partial r_i} = \lim_{\Delta r_i \to 0} \frac{\phi(r_i + \Delta r_i) - \phi(r_i)}{\Delta r_i}$$

$$\left(\frac{\partial \phi}{\partial r_j(i)}\right) \approx \frac{\phi(i-1) - \phi(i}{r_j(i-1) - r_j(}$$

Approximations



- **Backward difference scheme(BDS)**

$$\left(\frac{\partial \phi}{\partial r_j(i)}\right) = \frac{\phi(i) - \phi(i-1)}{r_j(i) - r_j(i-1)}$$

- **Central difference scheme (CDS)**

$$\left(\frac{\partial \phi}{\partial r_j(i)}\right) = \frac{\phi(i+1) - \phi(i-1)}{r_j(i+1) - r_j(i-1)}$$

- **Forward difference scheme (FDS)**

$$\left(\frac{\partial \phi}{\partial r_j(i)}\right) = \frac{\phi(i+1) - \phi(i)}{r_j(i+1) - r_j(i)}$$

Finite difference method – higher derivatives

- **2nd order - CDS between $r_j(i-1/2)$, $r_j(i+1/2)$:**

$$\left(\frac{\partial \phi}{\partial r_j(i+1/2)}\right) = \frac{\phi(i+1) - \phi(i)}{r_j(i+1) - r_j(i)}$$

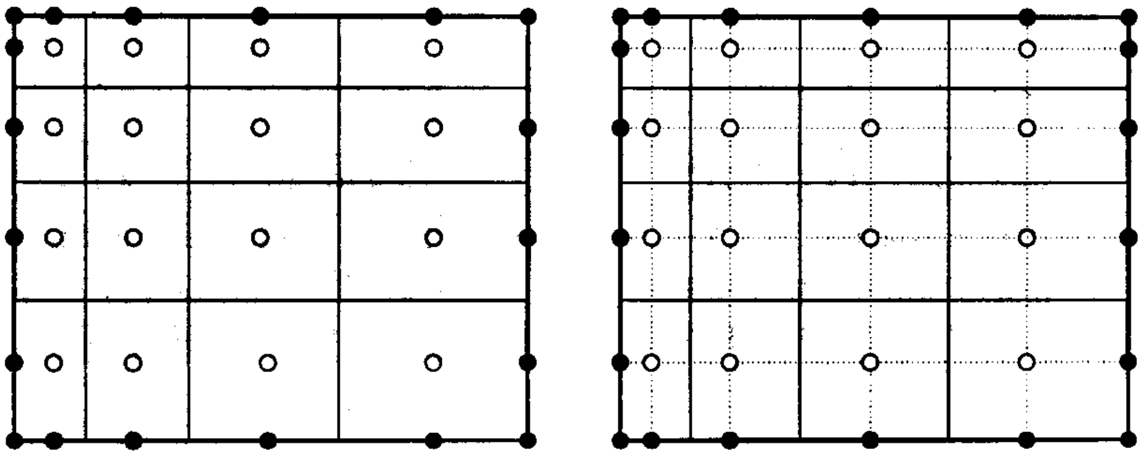
$$\left(\frac{\partial \phi}{\partial r_j(i-1/2)}\right) = \frac{\phi(i) - \phi(i-1)}{r_j(i) - r_j(i-1)}$$

$$\left(\frac{\partial \phi}{\partial r_j(i)}\right) = \frac{\left(\frac{\partial \phi}{\partial r_j(i+1/2)}\right) - \left(\frac{\partial \phi}{\partial r_j(i-1/2)}\right)}{\left[r_j(i+1) - r_j(i-1)\right]/2}$$

$$= \frac{\phi(i+1)\left[r_j(i) - r_j(i-1)\right] + \phi(i-1)\left[r_j(i+1) - r_j(i)\right] - 2\phi(i)\left[r_j(i+1) - 2r_j(i) + r_j(i-1)\right]}{\left[r_j(i+1) - r_j(i-1)\right]\left[r_j(i+1) - r_j(i)\right]\left[r_j(i) - r_j(i-1)\right]/2}$$

Finite volume method

- **Full system is divided into control volumes (CV)**



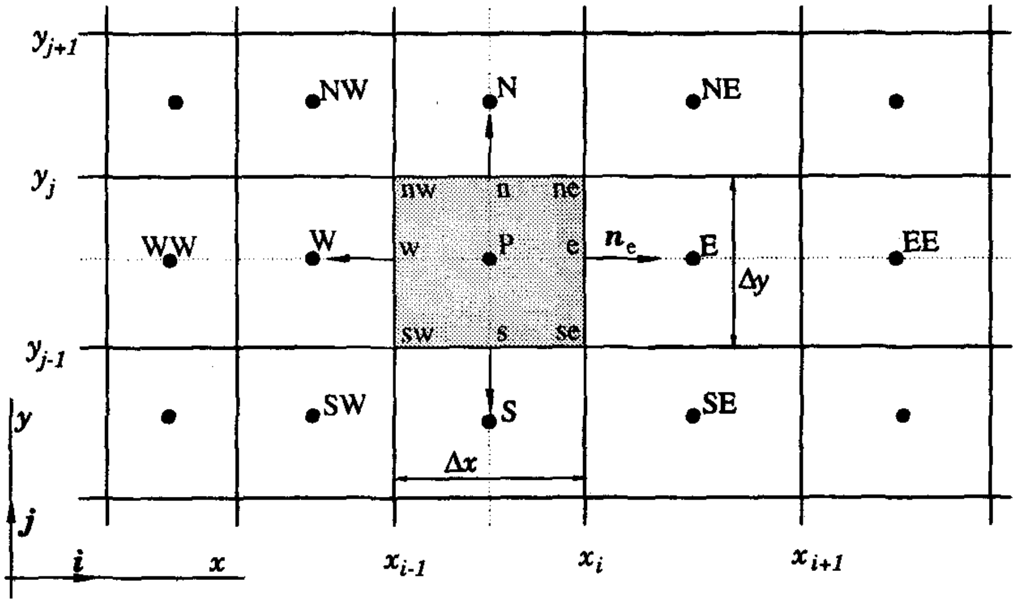
Different relations between mesh sites and CV:

Left – on the center of CV

Right – walls centered between the sites

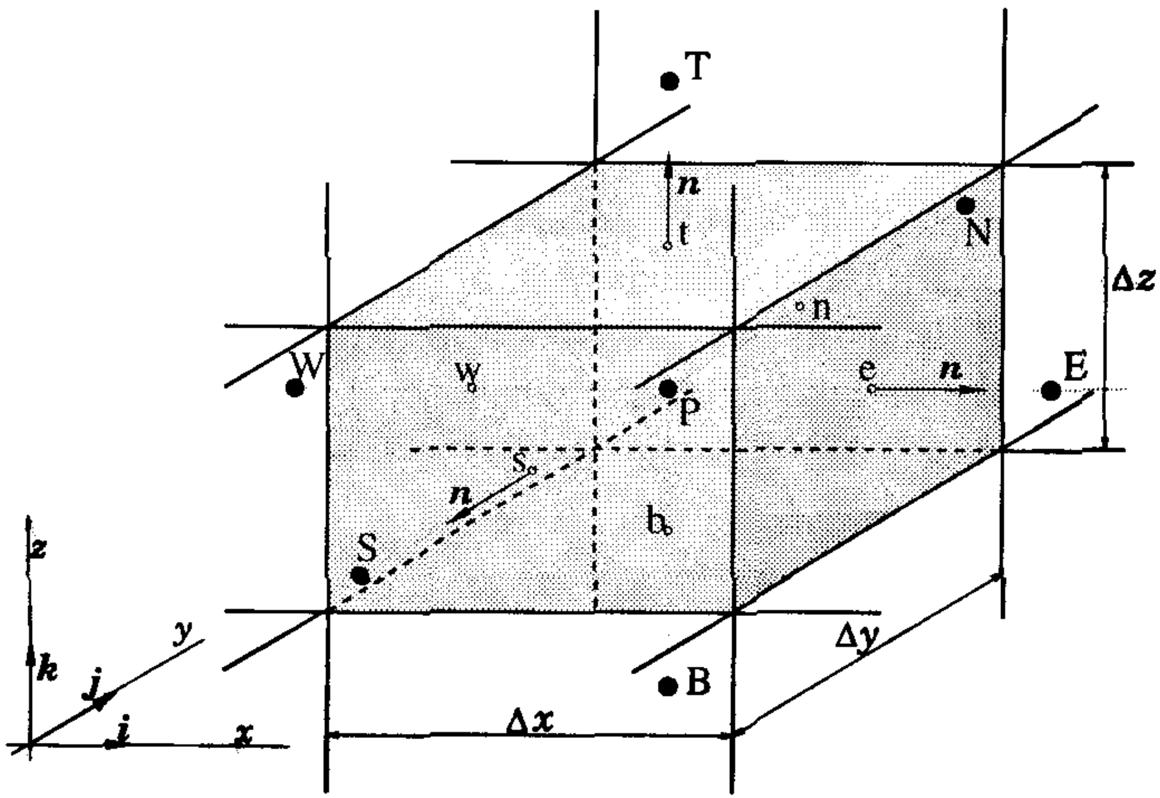
Finite volume method – implementation 2D

- **Field values are determined in the center only**



Definition of CV and notation in 2-d Cartesian mesh

Finite volume method– implementation 3D



Definition of CV and notation in 3-d Cartesian mesh

Finite volume method - integration

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(v_i\rho\phi)}{\partial r_i} = \frac{\partial}{\partial r_j}\left[\Gamma\frac{\partial\phi}{\partial r_j}\right] + q_\phi \qquad \frac{\partial(v_i\rho\phi)}{\partial r_i} = \frac{\partial}{\partial r_j}\left[\Gamma\frac{\partial\phi}{\partial r_j}\right] + q_\phi$$

- **Equation of motion are integrated over CV**

$$\int_S \rho\phi(\vec{v}\cdot\vec{n})d^2r = \int_S \phi(\nabla\phi\cdot\vec{n})d^2r + \int_V s_\phi d^3r$$

- **Surface integrals**

$$\int_{S_e} f d^2r = f_e S_e$$

- **Volume integrals**

$$\int_\Omega q d^3r = q_p\Omega$$

Finite element method (FEM) - properties

- **Strong differential & weak integral equations are equivalent**
- **Weak form – any function w(r,t)**

Solution – sum (combination) of functions defined on the element (any shape)

- **Interpolation function – any field value**
- **Interpolation function – any gradient value**
- **Field – continuous function of the coordinates**

Finite element method (FEM)

- **Equation of motion - differential form**

$$\frac{\partial}{\partial r_j}\left[\Gamma \frac{\partial \phi}{\partial r_j}\right] + q_\phi = 0$$

- **Equation of motion – integral (weak) form (w – any function)**

$$\int_V w\left\{\frac{\partial}{\partial r_j}\left[\Gamma \frac{\partial \phi}{\partial r_j}\right] + q_\phi\right\} d^3r = 0$$

Green theorem gives

$$\int_S \left\{\left[w\Gamma n_j \frac{\partial \phi}{\partial r_j}\right]\right\} d^2r + \int_V \left\{w q_\phi - \frac{\partial w}{\partial r_j}\left[\Gamma \frac{\partial \phi}{\partial r_j}\right]\right\} d^3r = 0$$

Interpolation functions – linear (1-d & 2-d)

$$\phi(i_1) = \phi[x(i_1)] \qquad \phi(i_2) = \phi[x(i_2)]$$

- **Field in linear interpolation**

$$\phi(x) = \phi(i_1)\frac{x - x(i_2)}{x(i_1) - x(i_2)} + \phi(i_2)\frac{x - x(i_2)}{x(i_1) - x(i_2)} = \phi(i_1)u_{i_1}(x) + \phi(i_2)u_{i_2}(x)$$

- **Universal interpolation functions**

$$u_{i_1}(x) = \frac{x - x(i_2)}{x(i_1) - x(i_2)} \quad \Rightarrow \quad u_{i_1}(x_{i_1}) = 1 \qquad u_{i_1}(x_{i_2}) = 0$$

$$u_{i_2}(x) = \frac{x - x(i_1)}{x(i_1) - x(i_2)} \quad \Rightarrow \quad u_{i_1}(x_{i_1}) = 0 \qquad u_{i_1}(x_{i_2}) = 1$$

Interpolation functions – linear (2-d)

$\phi(i_1,) = \phi[x(i_1)]$ $\phi(i_2) = \phi[x(i_2)]$

- **Field in linear interpolation**

$$\phi(x) = \phi(i_1)\frac{x - x(i_2)}{x(i_1) - x(i_2)} + \phi(i_2)\frac{x - x(i_2)}{x(i_1) - x(i_2)} = \phi(i_1)u_{i_1}(x) + \phi(i_2)u_{i_2}(x)$$

- **Universal interpolation functions**

$$u_{i_1}(x) = \frac{x - x(i_2)}{x(i_1) - x(i_2)} \Rightarrow u_{i_1}(x_{i_1}) = 1 \quad u_{i_1}(x_{i_2}) = 0$$

$$u_{i_2}(x) = \frac{x - x(i_1)}{x(i_1) - x(i_2)} \Rightarrow u_{i_1}(x_{i_1}) = 0 \quad u_{i_1}(x_{i_2}) = 1$$

Interpolation functions – linear (2-d)

$$\phi(i_1, j_1) = \phi[x(i_1), y(j_1)] \qquad \phi(i_2, j_1) = \phi[x(i_2), y(j_1)]$$

$$\phi(i_1, j_2) = \phi[x(i_1), y(j_2)] \qquad \phi(i_2, j_2) = \phi[x(i_2), y(j_2)]$$

- **Field in linear interpolation**

$$\phi(x, y) = \phi(i_1, j_1)\frac{x - x(i_2)}{x(i_1) - x(i_2)}\frac{y - y(i_2)}{y(i_1) - y(i_2)} + .. = \phi(i_1, j_1)u_{i_1}(x)u_{i_1}(y) + \cdots$$

- **Universal interpolation functions**

$$u_{i_1}(x) = \frac{x - x(i_2)}{x(i_1) - x(i_2)} \qquad u_{j_1}(y) = \frac{y - y(j_2)}{y(j_1) - y(j_2)}$$

$$u_{i_2}(x) = \frac{x - x(i_1)}{x(i_1) - x(i_2)} \qquad u_{j_2}(y) = \frac{y - y(j_1)}{y(j_1) - y(j_2)}$$

Weight function w(r,t)

- **Approximate solution gives residue R**

$$\int_S \left\{\left[w\Gamma n_j \frac{\partial \phi}{\partial r_j}\right]\right\} d^2 r + \int_V \left\{w q_\phi - \frac{\partial w}{\partial r_j}\left[\Gamma \frac{\partial \phi}{\partial r_j}\right]\right\} d^3 r = \int_V R w d^3 r$$

- **Galerkin method – weight function is solution**

$$w(\vec{r}, t) = \phi(\vec{r}, t) = \sum c_i u_i(\vec{r}, t)$$

- **Additional condition – Residue is orthogonal to weight function**

$$\int_V R w d^3 r = 0$$

- **Final equation – array equation**

$$K\phi = f$$

Array equation

$$K\phi = f$$

$$\phi \sum_j \int_V d^3r \left[\Gamma\left(\nabla u_i \cdot \nabla u_j\right)\right]\phi(j) = \int_V d^3r\left[u_i\, q_\phi\right] + \int_S d^2r\, \{\vec{n} \cdot [u_i \Gamma \nabla(\phi)]\}$$

- **Rigidity matrix K:**

$$K_{ij} = \int_V d^3r\left[\Gamma\left(\nabla u_i \cdot \nabla u_j\right)\right]$$

- **Force vector f:**

$$f = f^s + f^b$$

- **Source vector f^s:**

$$f^s = \int_V d^3r\, \left[u_i \cdot q_\phi\right]$$

- **Boundary condition vector f^b:**

$$f^b = \int_S d^2r\, \{\vec{n} \cdot [u_i \nabla(\phi)]\}$$

Solution of nonlinear array equation – linear algebra

$$K(\phi)\phi = f$$

- **Initial solution - linear**

$K_o = K(\phi = 0)$ ⇨ $K_o\phi = f$ ⇨ $\phi = K_o^{-1}f$

- **SS –successive substitutions**

$K(\phi_0)\phi_1 = f$ ⇨ $\phi_1 = K^{-1}(\phi_0)f$ ⇨ $\phi_2 = K^{-1}(\phi_1)f$

- **Global methods: Newton-Raphson, Quasi-Newton**
- **Partial methods: Segregated solver**

- **Solution strategy (small system):**
  - **SS – first (slow convergence, extensive convergence radius)**
  - **QN, NR – finish (fast convergence, small convergence radius)**
- **Solution strategy (large system):**
  - **Segregated solver**

Convergence conditions

$$K(\phi)\phi = f$$

- **At any iteration (i), the following equation is fulfilled :**

$$K(\phi)\phi = f + r$$

r_i - residuum – of the norm:

$$R_i = \|r_i\| = \left(\sum_{\alpha} r_{\alpha,i}^2\right)^{1/2}$$

$$\frac{\|R_i(\phi)\|}{\|R_o\|} \leq \varepsilon$$

- **Convergence criteria:**

Relative residuum measure

$$\frac{R_i}{R_o} \leq \varepsilon$$

Relative solution change in subsequent iterations

$$\frac{\|u_{i+1} - u_i\|}{\|u_i\|} \leq \varepsilon$$

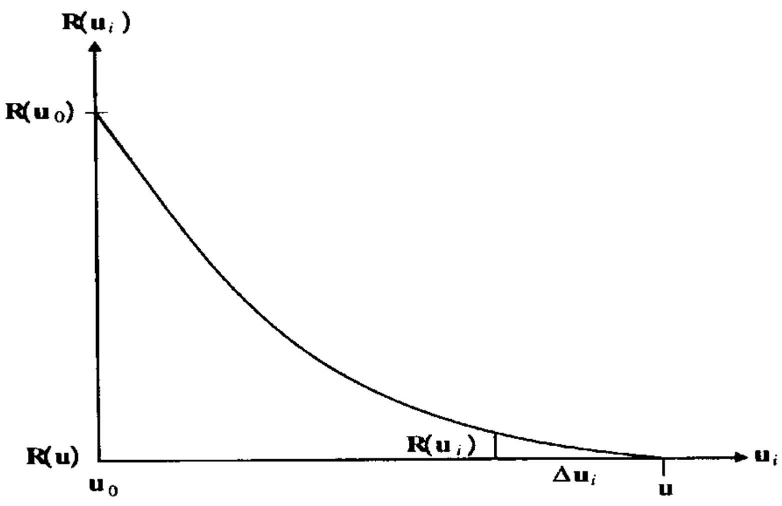
Types of convergence

- **Asymptotic convergence is defined as**:

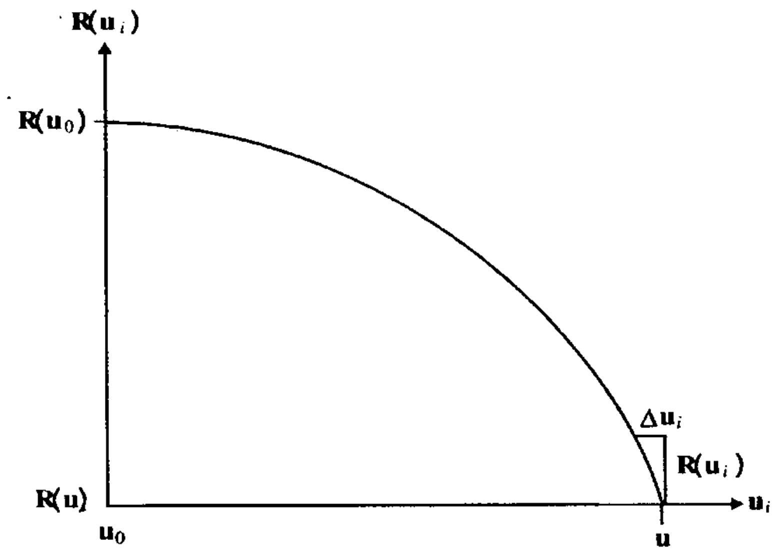
$$\left\|\phi_{i+1} - \phi_i\right\| \leq V \left\|\phi_i - \phi_{i-1}\right\|^k$$

k – convergence exponent: k=1 → linear (SS), k=2 → parabolic (NR, QN)

Residuum criterion



Relative change criterion



Example 1 : isothermal forced flow – gas mixer

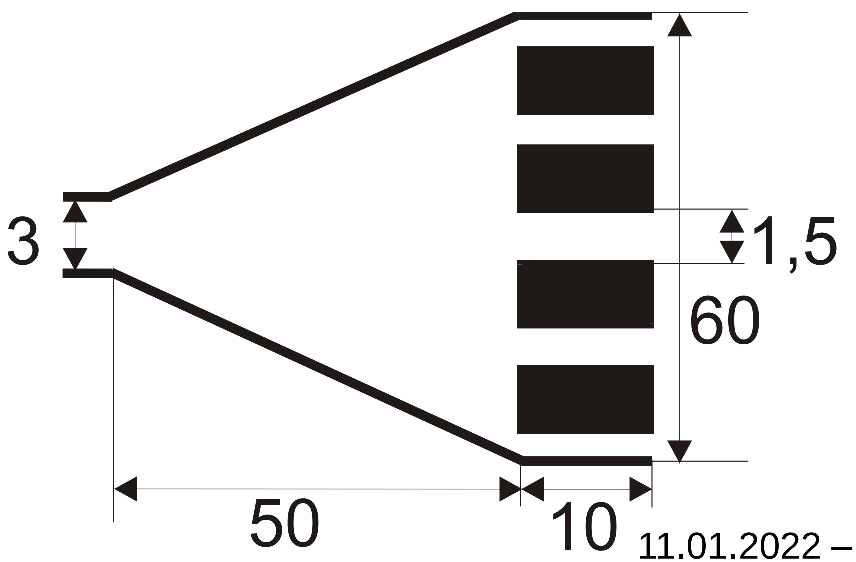
- **Equation motion isothermal incompressible fluid**:

$$div\left(\vec{v}(\vec{r},t)\right) = 0$$

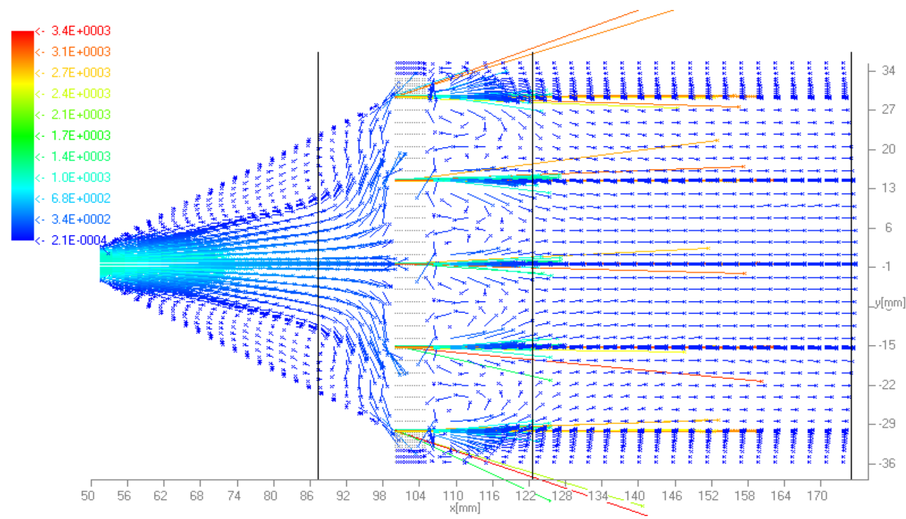
$$\rho_o\left[\frac{\partial \vec{v}(\vec{r},t)}{\partial t} + (\vec{v}(\vec{r},t)\cdot\nabla)\vec{v}(\vec{r},t)\right] = \mu\Delta\vec{v}(\vec{r},t)$$

- **Solid surfaces – no-slip condition:**

$$\vec{v}(\vec{r},t) = 0$$



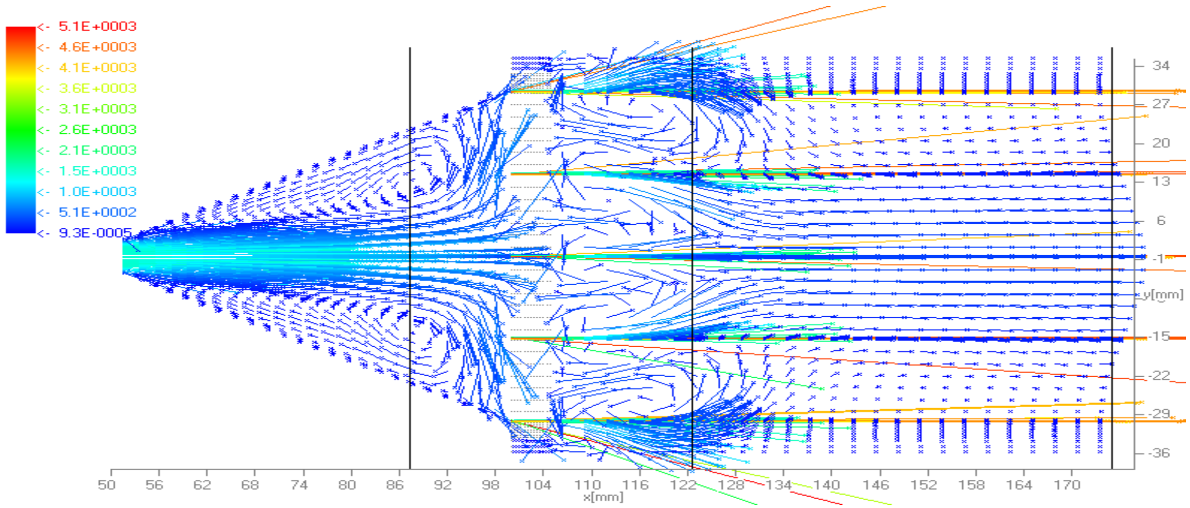
v = 1000 mm/s



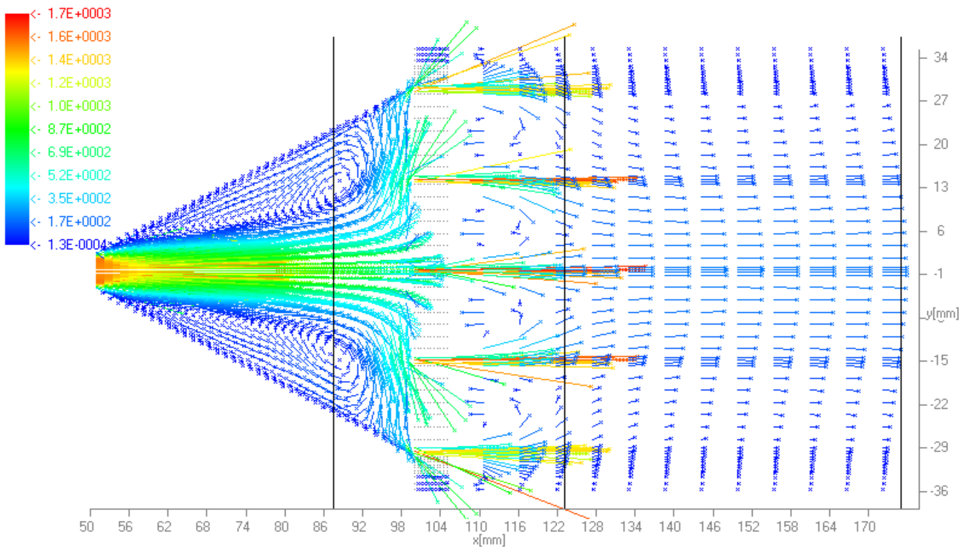
Michał Pawłowski – MSc thesis PD WUT (Fidap)

Isothermal forced flow – error

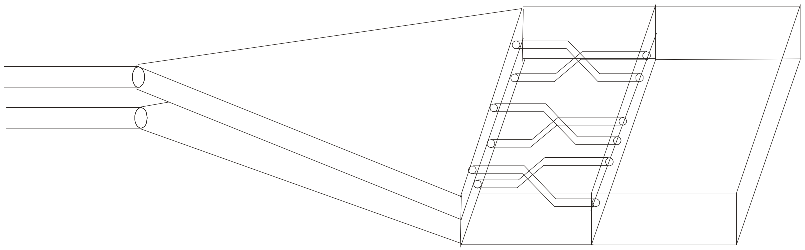
- **High flow – high error**

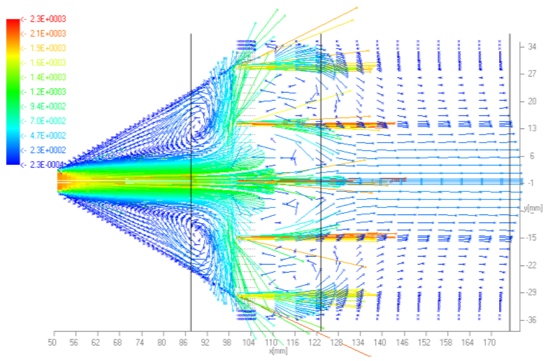


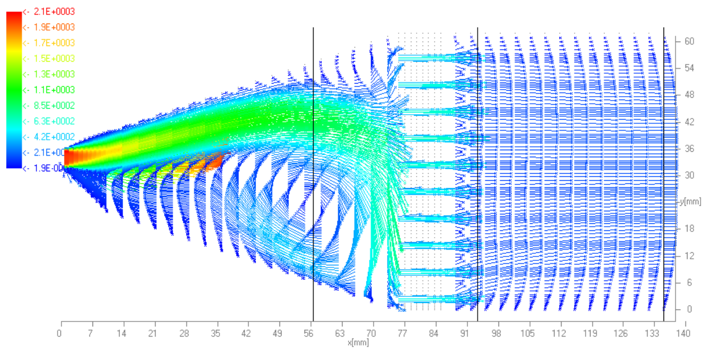
- **Small flow – small error**

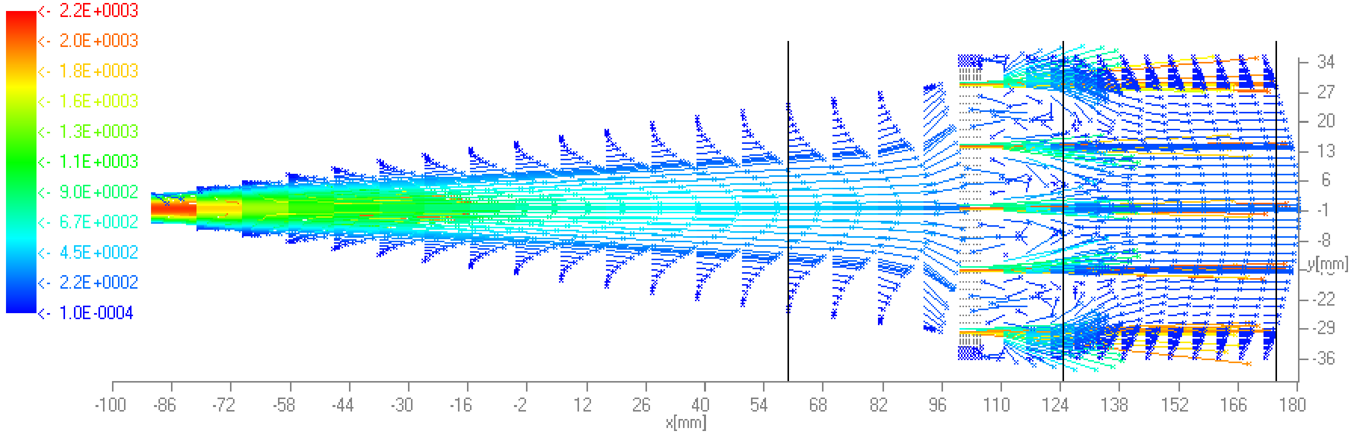


New design









2.2E+0003
2.0E+0003
1.8E+0003
1.6E+0003
1.3E+0003
1.1E+0003
9.0E+0002
6.7E+0002
4.5E+0002
2.2E+0002
1.0E-0004
34
27
20
13
6
-1
-8
y[mm]
-22
-29
-36
-100
-86
-72
-58
-44
-30
-16
-2
12
26
40
54
68
82
96
110
124
138
152
166
180
x[mm]

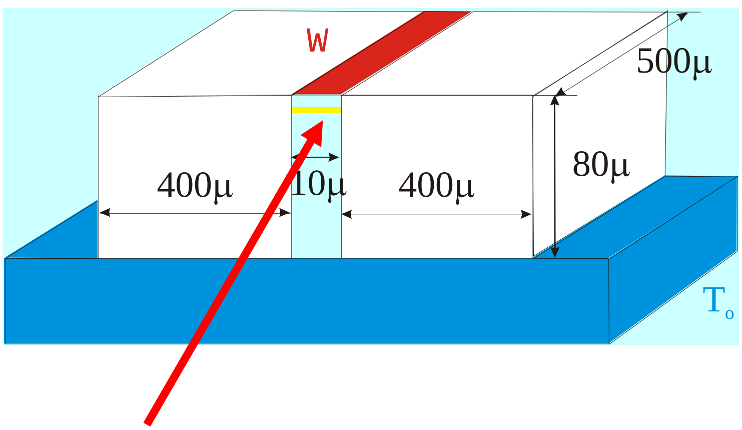
Blue laser temperature increase – heat conductivity

- **Outside heat generation zone**

$$C_p \frac{\partial[T(\vec{r},t)\rho(\vec{r},t)]}{\partial t} + \kappa\Delta T(\vec{r},t) = 0$$

- **Heat generation zone**

$$C_p \frac{\partial[T(\vec{r},t)\rho(\vec{r},t)]}{\partial t} + \kappa\Delta T(\vec{r},t) = j\rho$$



p-n junction

- **Boundary conditions: diamond chip**

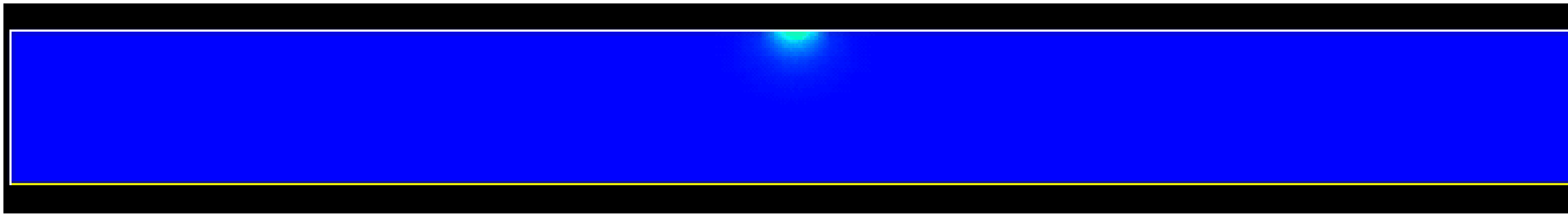
$$\boldsymbol{T = T_0}$$

- **Boundary conditions: other**

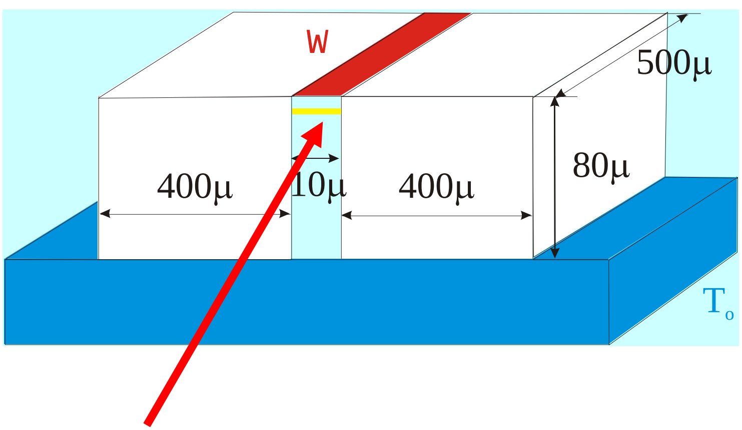
$$\boldsymbol{\vec{j}_q = -\kappa\nabla T = 0}$$

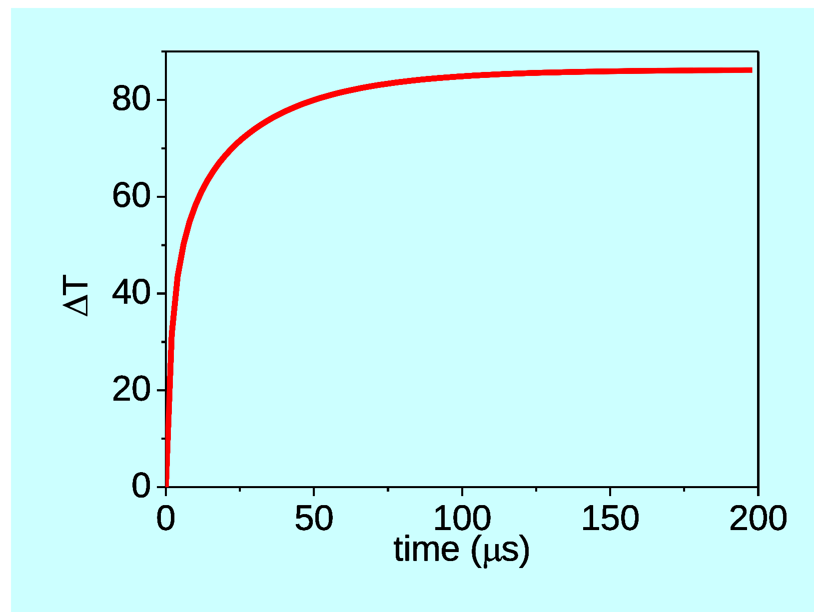
Stanisław Krukowski (Fidap)

Time evolution in IHPP laser diode



Power W = 12 W





p-n junction

Stanisław Krukowski (Fidap)

Natural convection in liquid Ga – GaN growth

- **Equation of motion**

$$div\left(\vec{v}(\vec{r},t)\right) = 0$$

$$\rho_o\left[\frac{\partial\vec{v}(\vec{r},t)}{\partial t} + (\vec{v}(\vec{r},t)\cdot\nabla)\vec{v}(\vec{r},t)\right] = \mu\Delta\vec{v}(\vec{r},t) + \rho_o[\beta_T(T-T_o)+\beta_c c]\vec{f}(\vec{r},t)$$

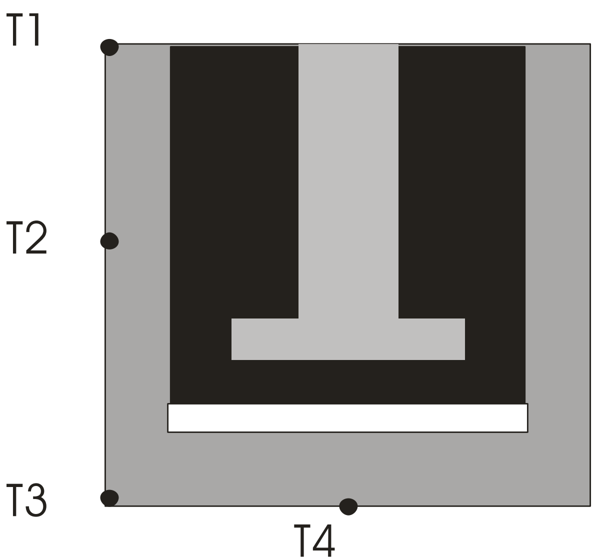
$$\rho_o C_p(T)\left[\frac{\partial[T(\vec{r},t)]}{\partial t} + (\vec{v}(\vec{r},t)\cdot\nabla)T(\vec{r},t)\right] = div\left(\kappa\nabla T(\vec{r},t)\right) + r_\varepsilon$$

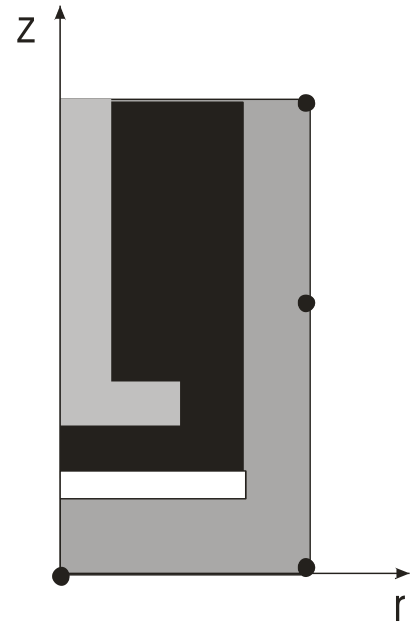
$$\vec{f}(\vec{r},t) = \vec{\boldsymbol{g}}$$

- **5 variables: 3 velocity components, pressure, temperature**
- **5 equations**
- **Additional equation:**

$$\boldsymbol{\rho} = \boldsymbol{\rho_o}$$

Natural convection – GaN crystal growth





- **Solid surfaces – no-slip condition velocity:**

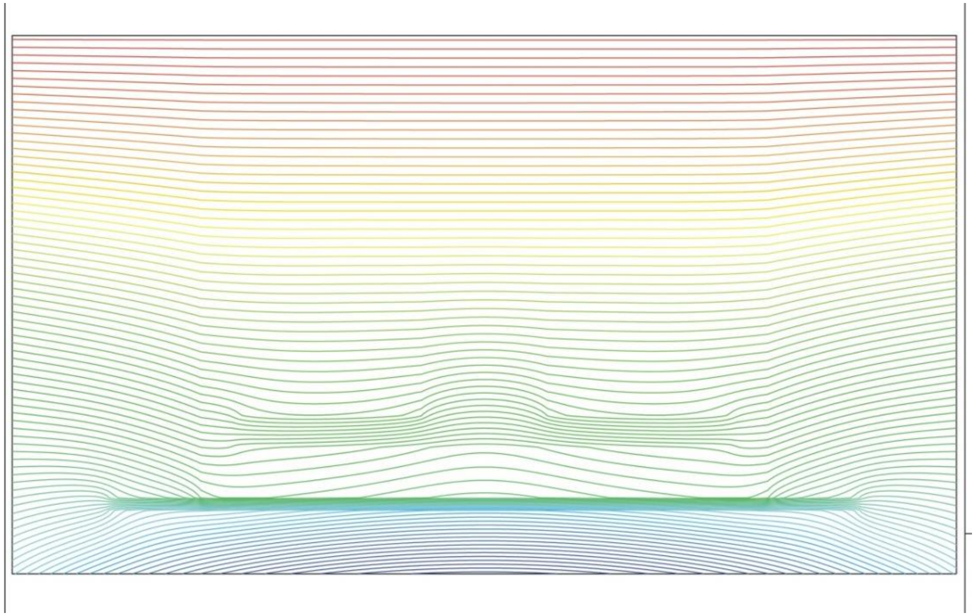
$$\vec{v}(\vec{r},t) = 0$$

- **Solid surfaces – temperature – from measurements:**

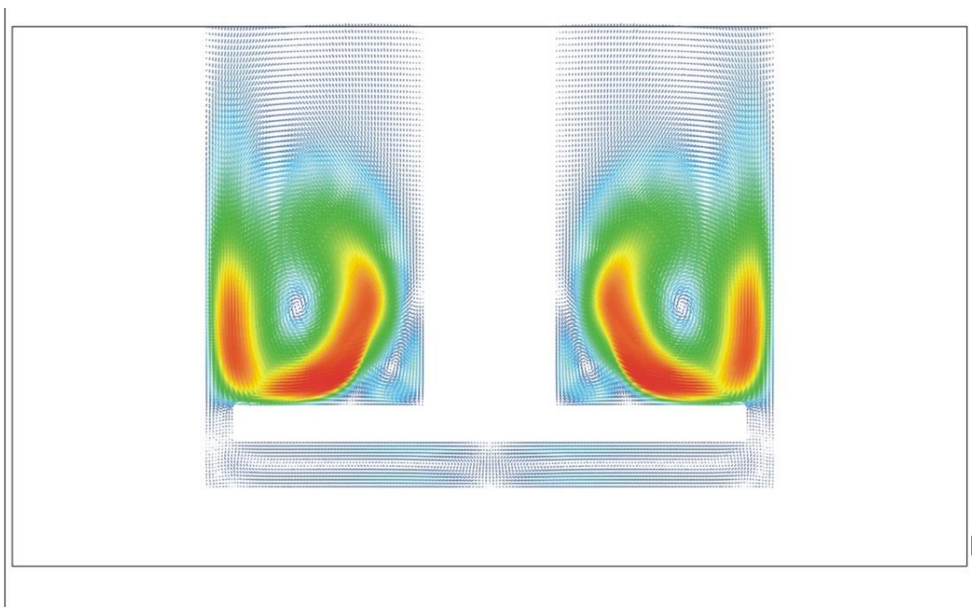
$$T(\vec{r},t) = T(\vec{r})$$

Paweł Strąk (Fidap)

Natural convection – GaN crystal growth



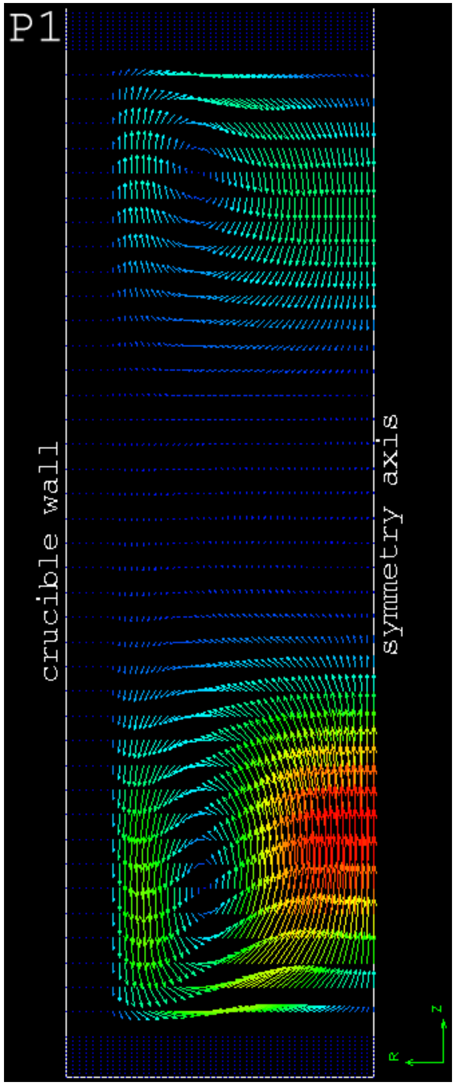
Temperature



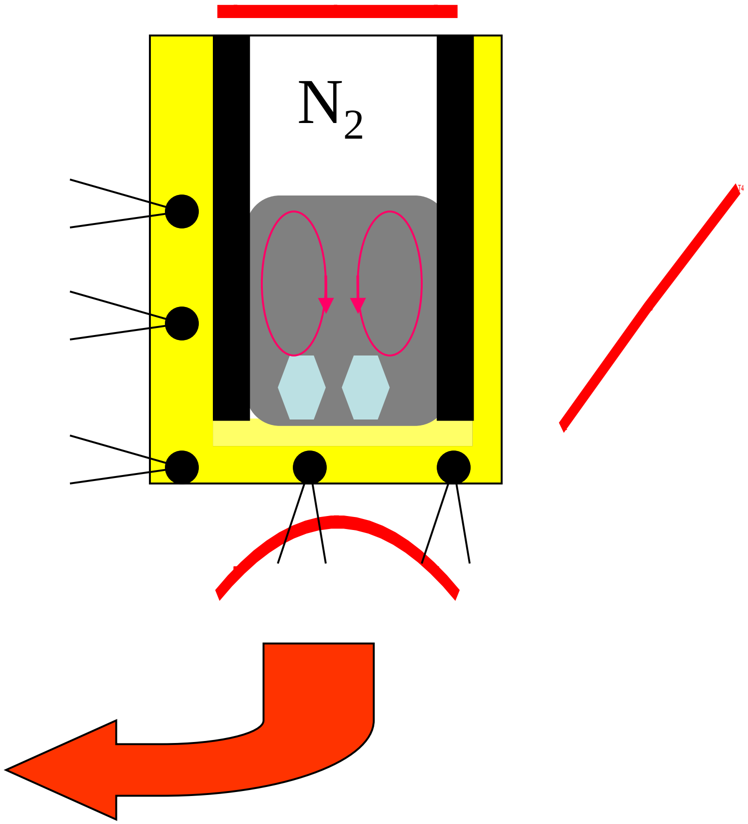
Velocity

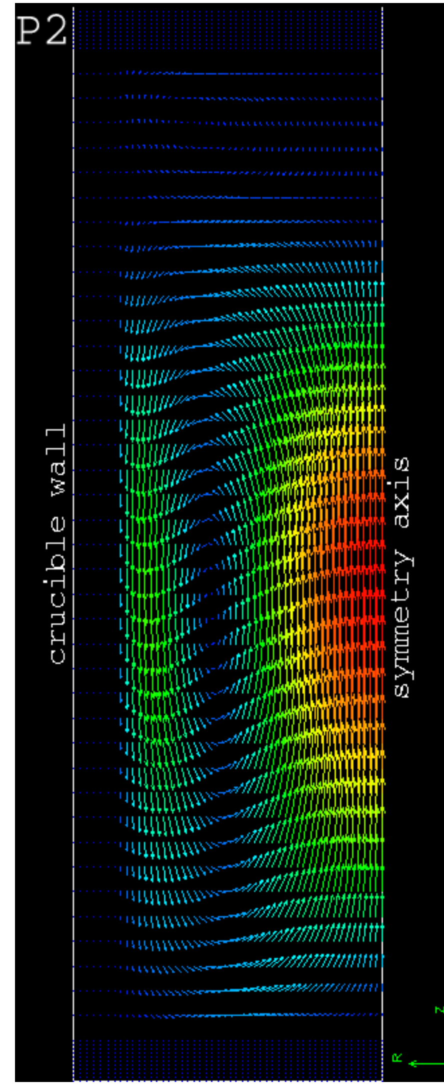
Paweł Strąk (Fidap)

Convection in gallium (Fidap)



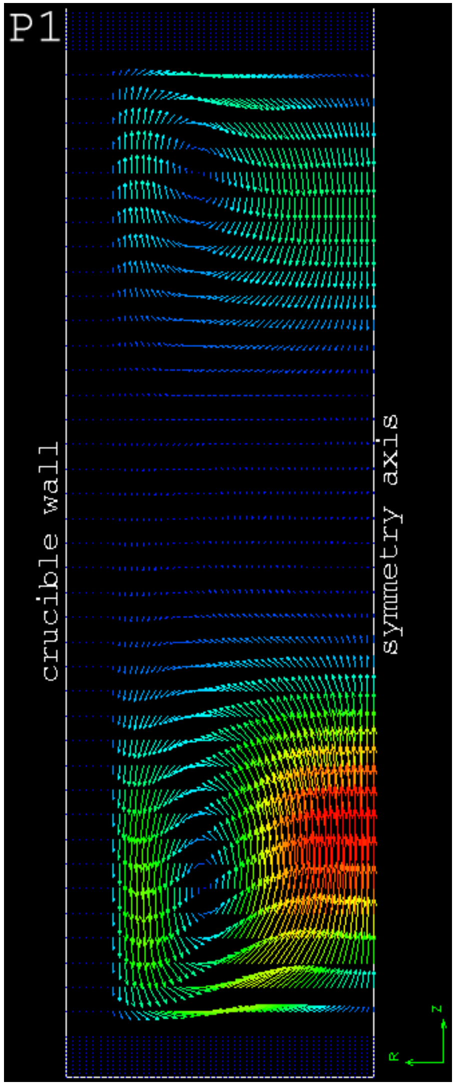
v_{max} = 0.96 mm/s



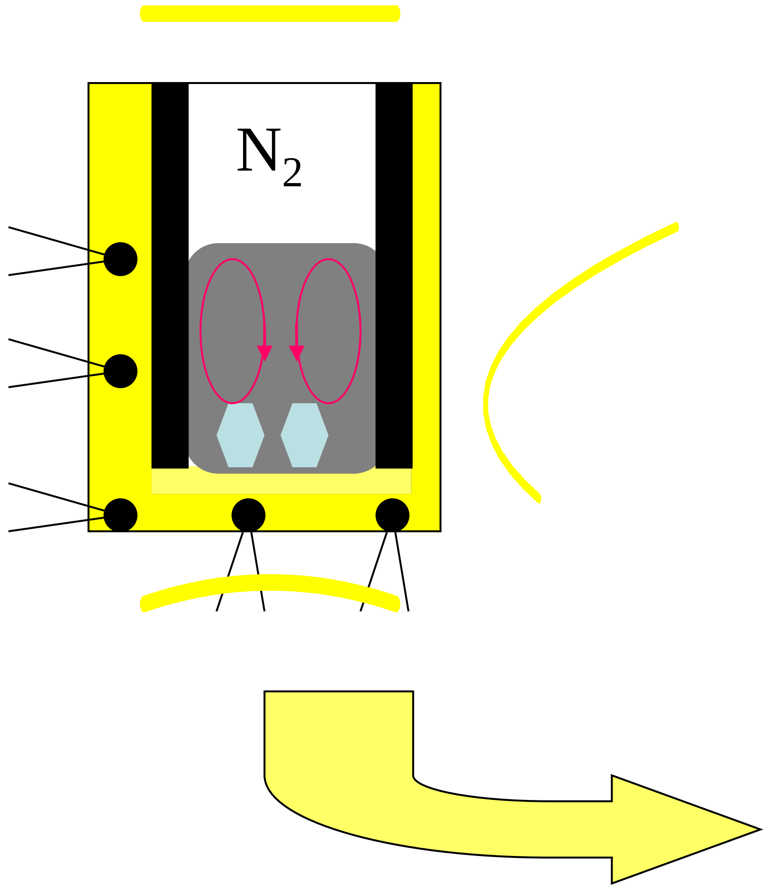


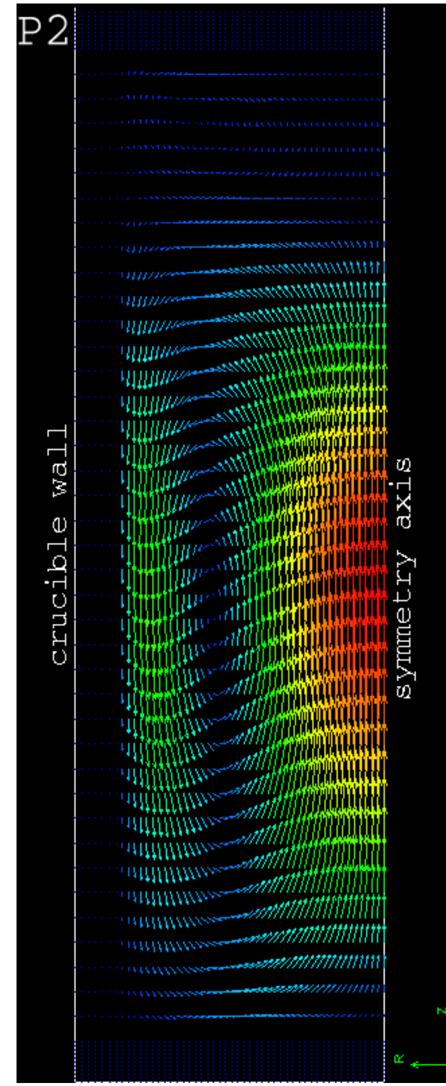
v_{max}= 3.57 mm/s

Convection in gallium (Fidap



v_{max} = 0.96 mm/s





v_{max} = 3.57 mm/s

Elasticity

- **Force equilibrium: f_i – bulk force**

$$\frac{\partial \sigma_{ij}}{\partial r_j} + f_i = 0$$

- **Hooke law: stress tensor σ_{ij} strain tensor u_{ij}:**

$$\sigma_{ij} = s_{ijkl}\, u_{kl}$$

- **Strain tensor and vector**

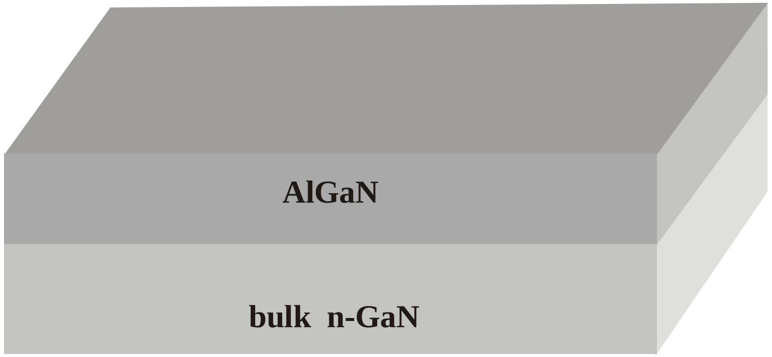
$$u_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial r_l} = \frac{\partial u_l}{\partial r_k}\right)$$

- **Linear elasticity equations**

$$s_{ijkl}\left(\frac{\partial^2 u_k}{\partial r_j \partial r_l} + \frac{\partial^2 u_l}{\partial r_j \partial r_k}\right) + 2f_i = 0$$

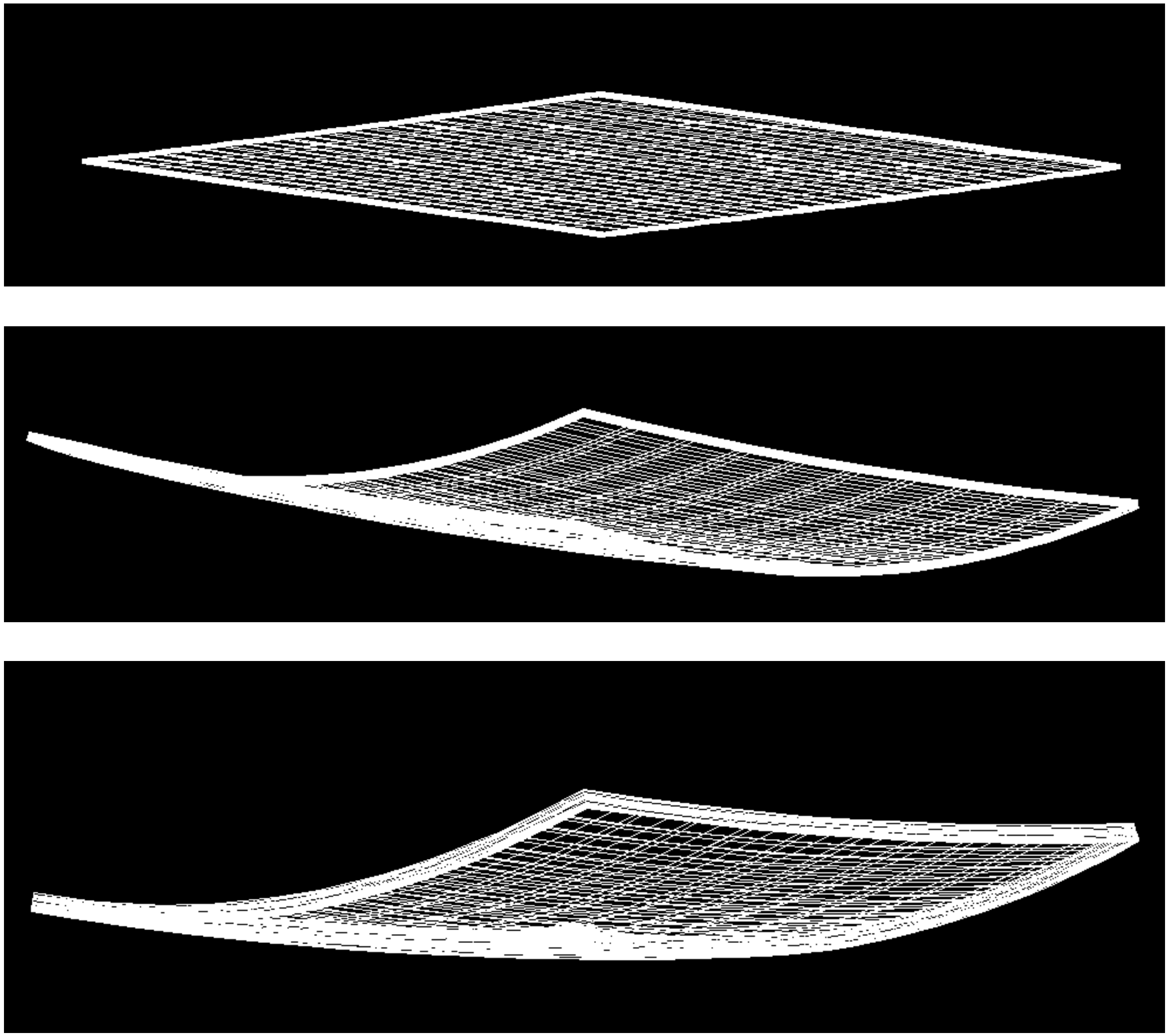
Strain in GaN laser - Abaqus

- 2-layer structure
- Fully strained
- Wegard law for lattice constants
- Elastic anisotropic approach



http://www.simulia.com/

Bowing in GaN/AlGaN structure - FEM



h = 1 μm

h = 50 μm

h = 180 μm

Substrate:

Thickness H = 60 μm

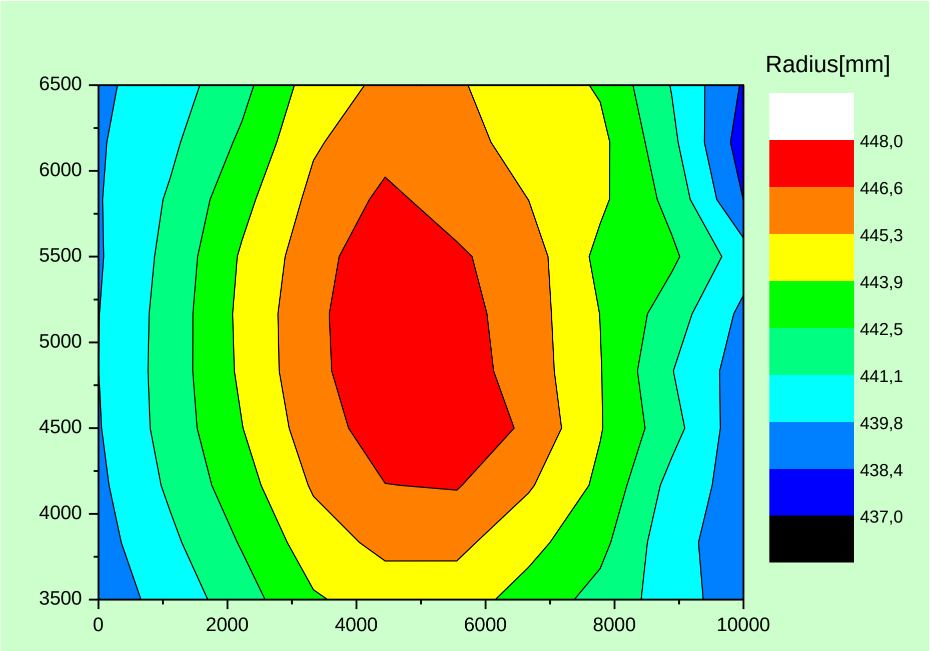
Size – 1cm x 1cm

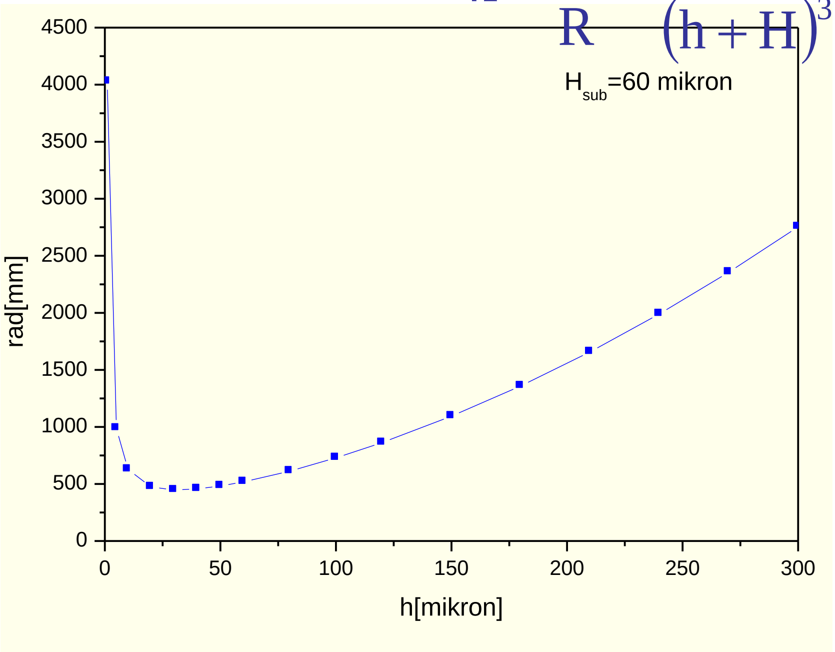
Magnification factor - 100

Calculations – S. Krukowski/Abaqus

Curvature radii - surface

$$\kappa = \frac{1}{R} = \frac{6fH}{(h+H)^3}$$





Clyne formula

$$\kappa = \frac{1}{R} = \frac{6\,f\,H}{(h+H)^2}$$

Stoney formula (dla h/H < 0.05)

$$\kappa = \frac{1}{R} = \frac{6\,f}{H}$$

$E_{layer} = E_{substrate}$
f – misfit
h – layer thickness
H – substrate thickness

Good agreement with Stoney –Clyne theory

Acknowledgements for ICM UW

- **Access to commercial software**

  Fidap (ANSYS Inc.)

  Abaqus (Dassault Systèmes)

- **Computing facilities within G15-9 project**