Introducing a New Product

Title

Sistem enacb

◆ Sistem:

Poissonova: $\Delta\phi=-\dfrac{\rho}{\epsilon\epsilon_0}$

kontinuitetni: $0=-\dfrac{\nabla J_n}{-e_0}+U$

$0=-\dfrac{\nabla J_p}{e_0}+U$

tokovi: $J_n=e_0\left[n\mu_n\left(-\nabla\phi\right)+D_n\nabla n\right]$

$J_p=e_0\left[p\mu_p\left(-\nabla\phi\right)-D_p\nabla p\right],\ D_{n,p}=\dfrac{k_BT}{e_0}\mu_{n,p}$

nosilci naboja: $n=n_i\mathrm{e}^{\left[\frac{e_0}{k_BT}\left(\varphi_n-\psi\right)\right]}$

$p=n_i\mathrm{e}^{\left[\frac{e_0}{k_BT}\left(\psi-\varphi_p\right)\right]}$

◆ Brezdimenzijska oblika:

$\dfrac{x}{a}\ \rightarrow\ x,\qquad \psi\dfrac{e_0}{k_BT}\ \rightarrow\ \psi,\qquad \phi_{p,n}\dfrac{e_0}{k_BT}\ \rightarrow\ \phi_{p,n}$

$$\nabla^2\psi=A\left[n_i(\tilde{p}-\tilde{n})+N_{shalow}+\sum_{t,don.}\left(1-P_t\right)N_t-\sum_{t,akc.}P_tN_t\right],$$

$$\Delta\varphi_n+\nabla\varphi_n\left(\nabla\varphi_n-\nabla\psi_n\frac{\nabla\mu_n}{\mu_n}\right)=-C\frac{U}{\tilde{n}\mu_n},$$

$$\Delta\varphi_p+\nabla\varphi_p\left(\nabla\varphi_p-\nabla\psi_p\frac{\nabla\mu_p}{\mu_n}\right)=-C\frac{U}{\tilde{p}\mu_p}$$

RP: $\nabla^2\psi_{x=0,1}=0$

$\varphi_n(1)=\varphi_p(1)=0,$

$\varphi_n(0)=\varphi_p(0)=\dfrac{e_0}{k_BT}V$

tokovi : $\dfrac{J_n}{e_0}=\dfrac{\mu_na}{C}\tilde{n}\nabla\varphi_n$

$\dfrac{J_p}{e_0}=\dfrac{\mu_pa}{C}\tilde{p}\nabla\varphi_p$

oznake:

$\tilde{p}=\mathrm{e}^{\psi-\varphi_p}$ $\qquad \tilde{n}=\mathrm{e}^{\varphi_n-\psi}$

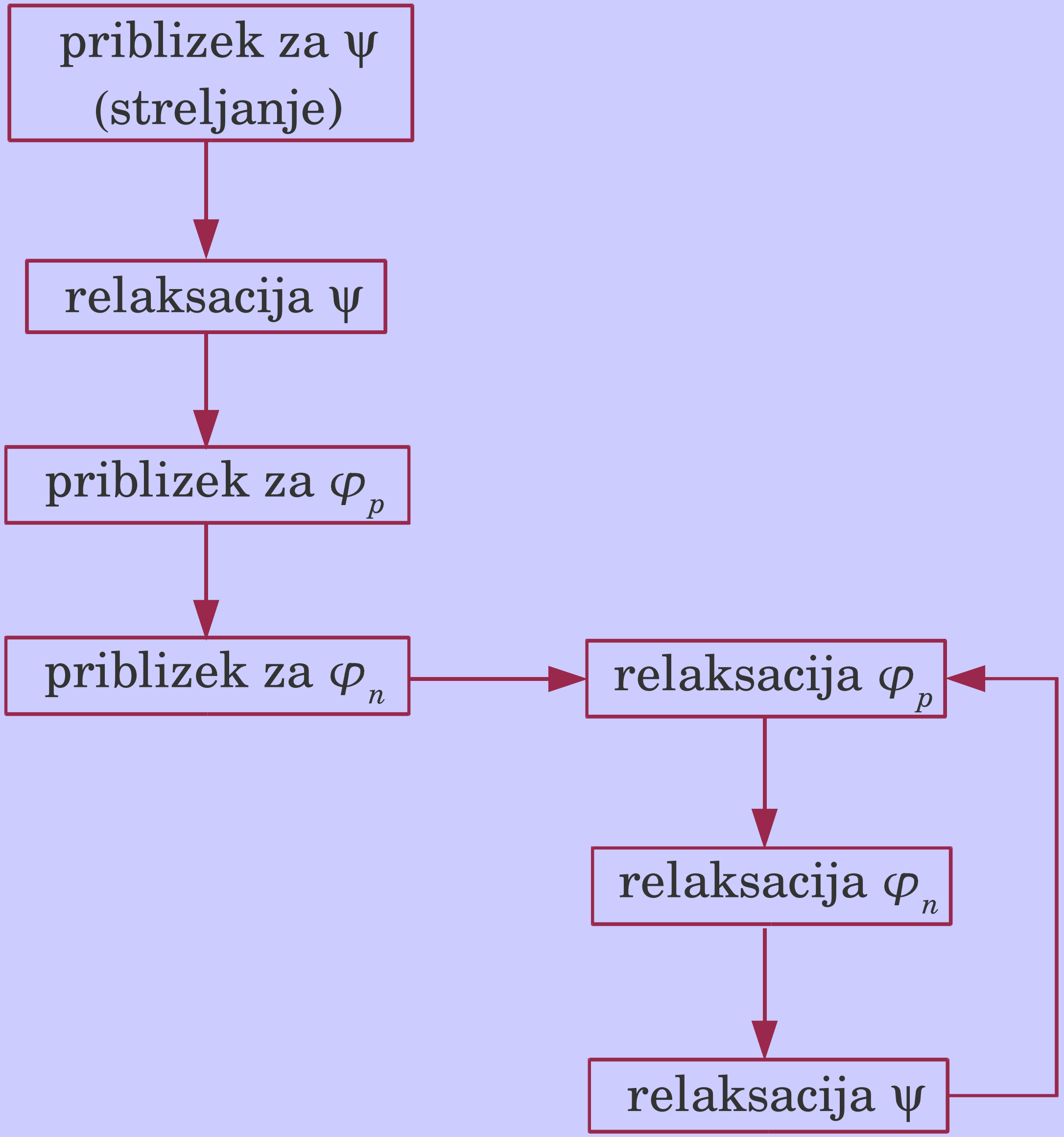
$C=\dfrac{e_0a^2}{k_BTn_i}$ $\qquad A=\dfrac{e_0^2a^2}{k_BT\epsilon\epsilon_0}$

$P_t=\dfrac{1+\tilde{n}B_t}{1+\tilde{n}B_t+\chi_t\left(\tilde{p}+B_t\right)}$

$\chi_t=\mathrm{e}^{\frac{E_t-E_i}{k_BT}}$ $\qquad \theta_t=\dfrac{v_{th}^n\sigma_t^n}{v_{th}^p\sigma_t^p}$

$B_t=\chi_t/\theta_t$

Postopek



priblizek za ψ (streljanje)

relaksacija ψ

priblizek za φ_p

priblizek za φ_n

relaksacija φ_p

relaksacija φ_n

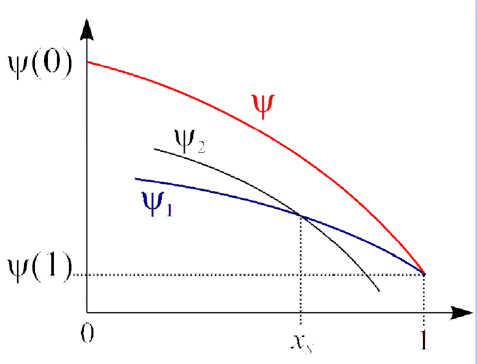
relaksacija ψ

Priblizek za ψ

- Resevanje $\nabla^2\psi = \overbrace{A[n_i(\tilde{p}-\tilde{n}) + N_{shalow} + \sum_{t,don.}\left(1-P_t\right)N_t - \sum_{t,akc.} P_t N_t]}^{f},\quad$ RP: $\nabla^2\psi_{x=0,1}=0$
  - Integrator Runge_Kutta 4
  - streljanje iz tocke $0<x_s<1$, kako do $\psi(x_s)$, $\nabla\psi(x_s)$?
    - ⇒ velja $\frac{\partial f}{\partial \psi} > 0$, torej $\psi_1(x) > \psi_2(x) \Leftrightarrow \nabla^2\psi_1(x) > \nabla^2\psi_2(x)$
    - → ce se dve funkciji ψ_1 in ψ_2 sekata v neki tocki x_0, potem velja

$$\psi_1(x) > \psi_2(x) \Leftrightarrow \nabla\psi_1(x_0) > \nabla\psi_2(x_0), \qquad x > x_0$$

$$\psi_1(x) < \psi_2(x) \Leftrightarrow \nabla\psi_1(x_0) > \nabla\psi_2(x_0), \qquad x < x_0$$

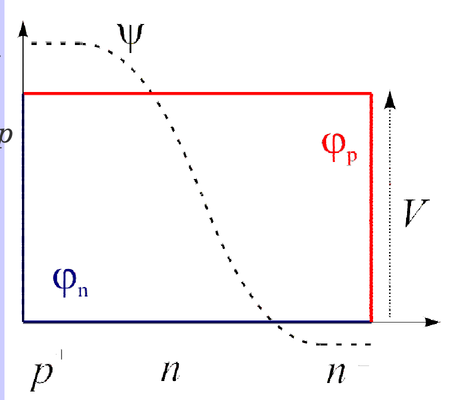


- Postopek
  - na robu je $\nabla^2\psi=0$ od tod dolocim (z bisekcijo) robni vrednosti $\psi(0)$ in $\psi(1)$;
  - ker je $\nabla\psi<0$, velja $\psi(0)< \psi(x)< \psi(1)$
  - pri danem $\psi(x_s)$ spreminjam $\nabla\psi(x_s)$ in streljam v desno:
    - ⇒ ce se med integracijo zgodi $\psi(x)<\psi(1)$, povecam odvod $\nabla\psi(x_s)$ "DOWN" resitev
    - ⇒ ce se med integracijo zgodi $\psi(x)>\psi(0)$, ali pa je na koncu $\psi>\psi(1)$ zmanjsam odvod $\nabla\psi(x_s)$ "UP" resitev
  - en strela v levo (z $\psi(x_s)$ in $\nabla\psi(x_s)$ iz zgornje tocke):
    - ⇒ ce se vmes zgodi $\psi(x)<\psi(1)$ ali pa je na koncu $\psi<\psi(0)$, povecam $\psi(x_s)$ "DOWN" resitev
    - ⇒ ce se zgodi $\psi(x)>\psi(0)$, zmanjsam $\psi(x_s)$ "UP" resitev

Priblizek za ψ

Vhodna vrednost
$\psi_s(x_s) = [\psi(0)\text{-}\psi(1)]/2$

Vhodna
φ_n in φ_p



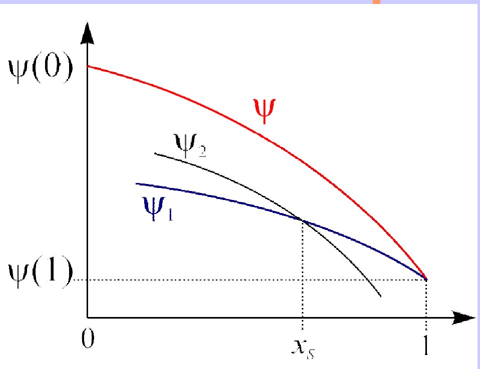
Iskanje $\nabla\psi_s$ in ψ_s v x_s

Iskanje $\nabla\psi_s$ z bisekcijo
pri danem ψ_s:

Iskanje zacetnih
$\nabla\psi_{DOWN}$ in $\nabla\psi_{UP}$ v x_s

Strel na desno v x_s z ψ_s in
$\nabla\psi_s = (\nabla\psi_{UP}\text{-}\nabla\psi_{DOWN})/2$
a) resitev UP: $\nabla\psi_s = \nabla\psi_{DOWN}$
b) resitev DOWN: $\nabla\psi_s = \nabla\psi_{UP}$

Strel na levo v x_s z $\nabla\psi_s$ in ψ_s
a) resitev UP: $\psi_s = \psi_{UP}$
b) resitev DOWN: $\nabla\psi_s = \nabla\psi_{DOWN}$
novi $\psi_s = (\psi_{UP}\text{-}\psi_{DOWN})/2$



Relaksacija ψ

- **Relaksacijska metoda**
  - poznamo priblizno resitev y za enacbo $\nabla^2 y \cong f(y)$
  - dodamo majhen popravek u: $y \to y+u$
  - za notranje tocke odvode nadomestim z diferencami, robni tocki pa zapisem tako, da zadostita robnima pogojema → sistem enacb $\mathbf{Au}=\mathbf{r}$

$$\left[\begin{array}{l} B_t = \chi_t / \theta_t \\ \dfrac{\partial f}{\partial \psi} = p + n \sum_t - \left(\dfrac{\partial P_t}{\partial \psi} \right) N_t \\ \dfrac{\partial P_t}{\partial \psi} = -\chi_t \dfrac{2 B_t \tilde{p} \tilde{n} + \tilde{p} + B_t^2 \tilde{n}}{\left[B_t \tilde{n} + 1 + \chi_t B_t \chi_t \tilde{p} \right]^2} \\ \chi_t = \exp\left(\dfrac{E_t - E_i}{k_B T} \right) \end{array}\right.$$

- **Resevanje** $\nabla^2 \psi = f$, RP: $\nabla^2 \psi_{x=0,1} = 0 \to \psi(0), \psi(1)$

$$\to \nabla^2 u - u \frac{\partial f}{\partial \psi} = f - \nabla^2 \psi$$

  - notranje tocke

$$\boxed{u_{k+1} \overbrace{\left[\frac{1}{h^2} \right]}^{c_k} + u_k \overbrace{\left[-\frac{2}{h^2} - \frac{\partial f}{\partial \psi} \right]}^{b_k} + u_{k-1} \overbrace{\frac{1}{h^2}}^{a_k} = \overbrace{f(\psi_k) - \frac{\psi_{k+1} - 2\psi_k + \psi_{k-1}}{h^2}}^{r_k}}$$

  - zunanje tocke ($k=0$ in $k=N$):

$$\boxed{\begin{array}{c} u_N = 0 \\ u_0 = 0 \end{array}}$$

  - tridiagonalni sistem →

$$\begin{bmatrix} b_0 & c_0 & \dots & & \\ a_1 & b_1 & c_1 & \dots & \\ & & \ddots & & \\ & \dots & a_{N-1} & b_{N-1} & c_{N-1} \\ & & \dots & a_N & b_N \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix} = \begin{bmatrix} r_0 \\ r_1 \\ \vdots \\ r_{N-1} \\ r_N \end{bmatrix}$$

Priblizka za φ_n φ_p

- elektroni

$$\frac{J_n}{e_0} = K'\mu_n I_n, \qquad I_n = \tilde{n}\nabla\varphi_n$$

$$\frac{\nabla J_n}{e_0} = -\frac{U}{d} \qquad \Big/ \int_0^x dy$$

$$I_n(x) = \frac{\mu_n(0)}{\mu_n(x)} I_n(0) - I_{gr}(x)$$

$$I_{gr}(x) = \frac{1}{\mu_n(x)} \int_0^x \frac{U(y)a}{K} dy$$

$$I_n(y) = \tilde{n}\nabla\varphi_n \qquad \Big/ e^{-\varphi_n(0)} \int_x^1 dy$$

$$\varphi_n(x) = \varphi_n(0) + \ln\left[e^{\varphi_n(1)-\varphi_n(0)} - A_n F_n(x) + FR_n(x)\right]$$

$$F_n(x) = \int_x^1 \frac{1}{\mu_n(y)} e^{\left(\psi(y)-\varphi_n(0)\right)} dy$$

$$FR_n(x) = \int_x^1 \frac{I_{gr}(y)}{\mu_n(y)} e^{\left(\psi(y)-\varphi_n(0)\right)} dy$$

$$A_n = \mu_n(0) I_n(0) = \frac{1}{F_n(0)}\left[e^{\left(\varphi_n(1)-\varphi_n(0)\right)} - 1 + FR_n(0)\right]$$

- vrzeli

$$\frac{J_p}{e_0} = K'\mu_p I_p, \qquad I_p = \tilde{p}\nabla\varphi_p$$

$$\frac{\nabla J_p}{e_0} = \frac{U}{d}$$

$$\varphi_p(x) = \varphi_p(1) - \ln\left[e^{\varphi_p(1)-\varphi_p(0)} - A_p F_n(x) - FR_p(x)\right]$$

$$F_p(x) = \int_0^x \frac{1}{\mu_p(y)} e^{\left(\varphi_p(0)-\psi(y)\right)} dy$$

$$FR_p(x) = \int_0^x \frac{I_{gr}(y)}{\mu_p(y)} e^{\left(\varphi_p(0)-\psi(y)\right)} dy$$

$$A_p = \mu_p(0) I_p(0) = \frac{1}{F_p(1)}\left[e^{\left(\varphi_p(1)-\varphi_p(0)\right)} - 1 - FR_p(1)\right]$$

Relaksacija φ_n

- Enacba:

$$\nabla\varphi_n+\nabla\varphi_n\left[\nabla\varphi_n-\nabla\psi+\frac{\nabla\mu_n}{\mu_n}\right]=-\underbrace{\frac{U}{D\tilde{n}\mu_n}}_{f_n},\qquad \text{RP:}\quad \varphi_n(x=1)=0,\quad \varphi_n(x=0)=\frac{e_0}{k_B T}V$$

$$U=\sum_t N_t c_p^t n_i\left[\frac{1-\tilde{p}\tilde{n}}{\tilde{n}+\theta_t\tilde{p}+E_t}\right],\qquad \frac{\partial f_n}{\partial\varphi_n}=\sum_t\left[\alpha_t\frac{1+\tilde{p}\left(\tilde{p}\theta_t+E_t\right)}{\left(\tilde{n}+\theta_t\tilde{p}+E_t\right)^2}\right]-f_n$$

$$E_t=\chi_t+\theta_t/\chi_t$$

$$\alpha_t=\frac{N_t c_p^t a^2 e_0}{k_B T\mu_n}$$

$$D=\frac{k_B T n_i}{a^2 e_0}$$

- Odvodi → diference:
  - notranje tocke x_k

$$\boxed{\begin{aligned}
&u_{k+1}\overbrace{\left[\frac{1}{h^2}+\frac{1}{2h}G_k\right]}^{c_k}+u_k\overbrace{\left[-\frac{2}{h^2}-\frac{\partial f_n}{\partial\varphi_n}\right]}^{b_k}+u_{k-1}\overbrace{\left[\frac{1}{h^2}-\frac{1}{2h}G_k\right]}^{a_k}=r_k\\
&r_k=f_n(x_k)-\nabla^2\varphi_n(x_k)+\nabla\varphi_n(x_k)\left(-\nabla\varphi_n(x_k)+\nabla\psi-\frac{\nabla\mu_n}{\mu_n}\right)\\
&G_k=2\nabla\varphi_n(x_k)-\nabla\psi(x_k)+\frac{\nabla\mu_n(x_k)}{\mu_n(x_k)}
\end{aligned}}$$

  - zunanje tocke $u_0=0$

    $u_N=0$

Relaksacija φ_p

- Enacba:

$$\nabla^2\varphi_p+\nabla\varphi_p\left[-\nabla\varphi_p+\nabla\psi+\frac{\nabla\mu_p}{\mu_p}\right]=\underbrace{-\frac{U}{D\,\tilde{p}\,\mu_p}}_{f_p},\qquad \text{RP:}\quad \varphi_p(x=1)=0,\quad \varphi_p(x=0)=\frac{e_0}{k_BT}V$$

$$U=\sum_t N_t c_p^t n_i\left[\frac{1-\tilde{p}\,\tilde{n}}{\tilde{n}\,\theta_t\tilde{p}+E_t}\right],\qquad \frac{\partial f_n}{\partial\varphi_n}=\sum_t\left[\beta_t\frac{\theta_t+\tilde{n}\left(\tilde{n}+E_t\right)}{\left(\tilde{n}+\theta_t\tilde{p}+E_t\right)^2}\right]+f_p$$

$$E_t=\chi_t+\theta_t/\chi_t$$

$$\beta_t=\frac{N_t c_p^t a^2 e_0}{k_BT\mu_p}$$

$$D=\frac{k_BT\,n_i}{a^2 e_0}$$

- Odvodi → diference:
  - notranje tocke x_k

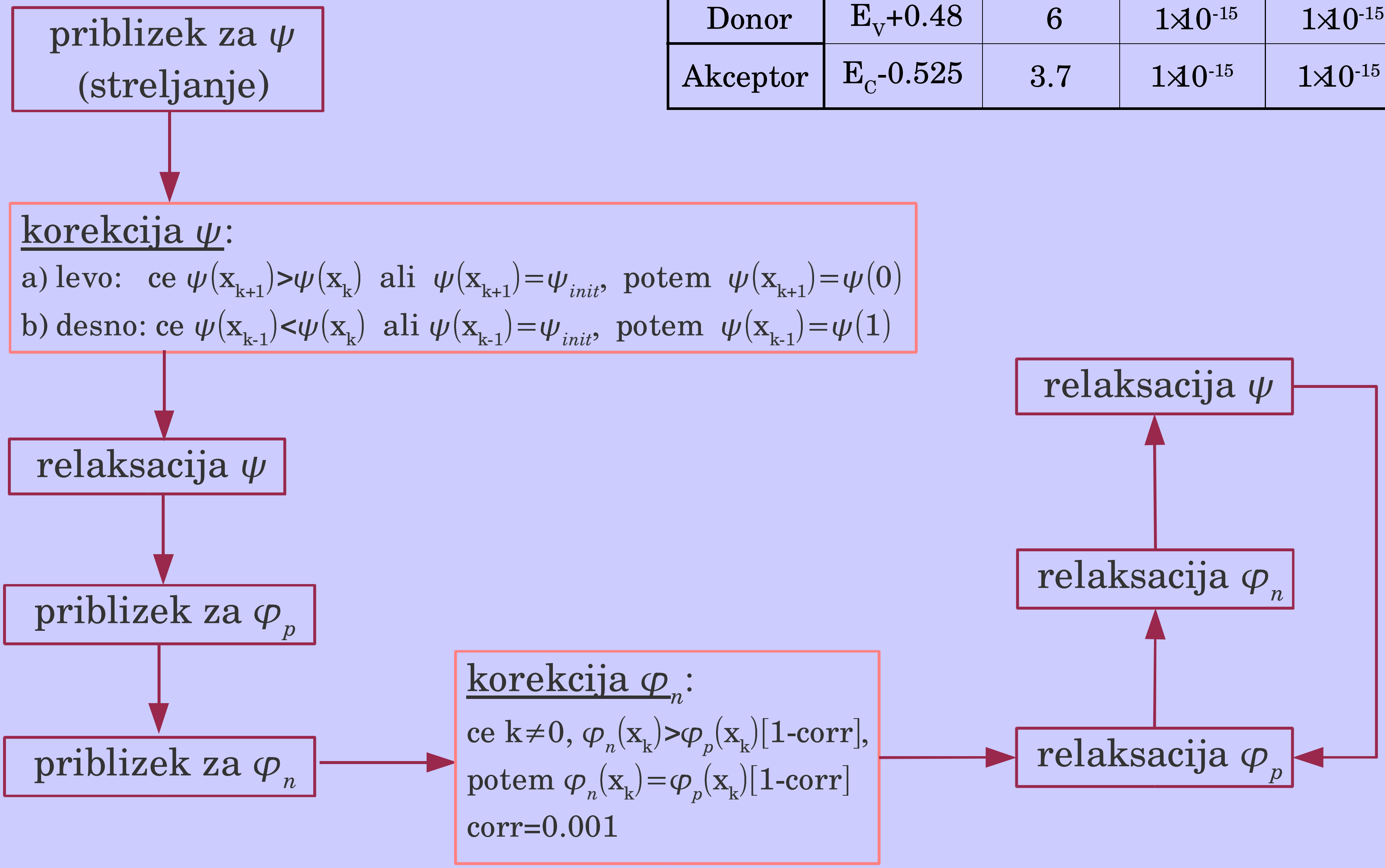
$$\boxed{\begin{aligned}
&u_{k+1}\overbrace{\left[\frac{1}{h^2}+\frac{1}{2h}G_k\right]}^{c_k}+u_k\overbrace{\left[-\frac{2}{h^2}-\frac{\partial f_p}{\partial\varphi_p}\right]}^{b_k}+u_{k-1}\overbrace{\left[\frac{1}{h^2}-\frac{1}{2h}G_k\right]}^{a_k}=r_k\\
&r_k=f_p(x_k)-\nabla^2\varphi_p(x_k)+\nabla\varphi_p(x_k)\left(\nabla\varphi_p(x_k)-\nabla\psi-\frac{\nabla\mu_p}{\mu_p}\right)\\
&G_k=-2\nabla\varphi_p(x_k)+\nabla\psi(x_k)+\frac{\nabla\mu_p(x_k)}{\mu_p(x_k)}
\end{aligned}}$$

  - zunanje tocke $u_0=0$
    $u_N=0$

Problemi

Parametri pasti:

PAST	E [eV]	g [1/cm]	σ_n [cm^{-2}]	σ_p [cm^{-2}]
Donor	E_V+0.48	6	1×10^{-15}	1×10^{-15}
Akceptor	E_C-0.525	3.7	1×10^{-15}	1×10^{-15}



priblizek za ψ (streljanje)

<u>korekcija ψ</u>:

a) levo: ce $\psi(x_{k+1})>\psi(x_k)$ ali $\psi(x_{k+1})=\psi_{init}$, potem $\psi(x_{k+1})=\psi(0)$

b) desno: ce $\psi(x_{k-1})<\psi(x_k)$ ali $\psi(x_{k-1})=\psi_{init}$, potem $\psi(x_{k-1})=\psi(1)$

relaksacija ψ

priblizek za φ_p

priblizek za φ_n

<u>korekcija φ_n</u>:

ce $k\neq0$, $\varphi_n(x_k)>\varphi_p(x_k)[1\text{-corr}]$,

potem $\varphi_n(x_k)=\varphi_p(x_k)[1\text{-corr}]$

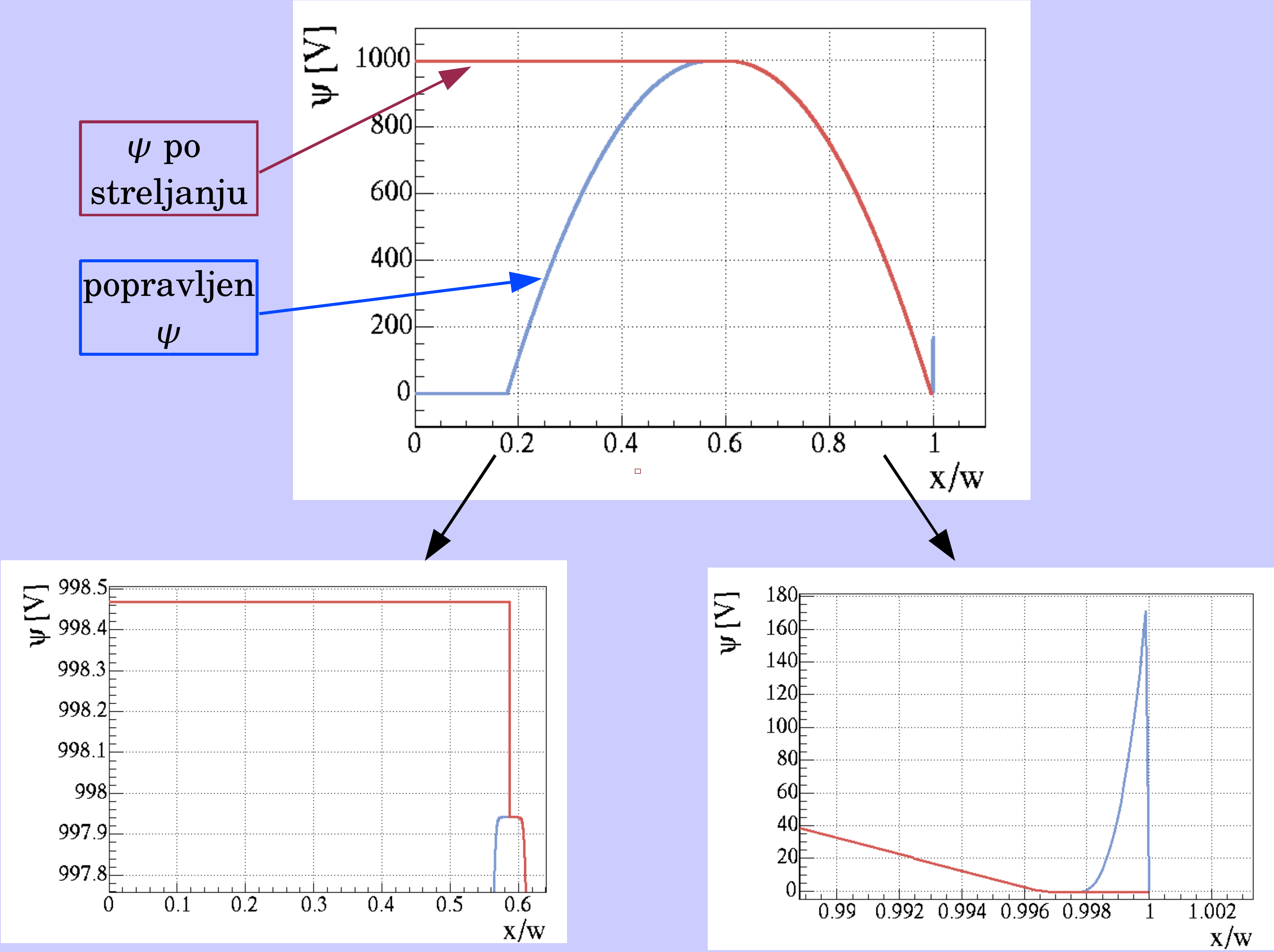
corr=0.001

relaksacija φ_p

relaksacija φ_n

relaksacija ψ

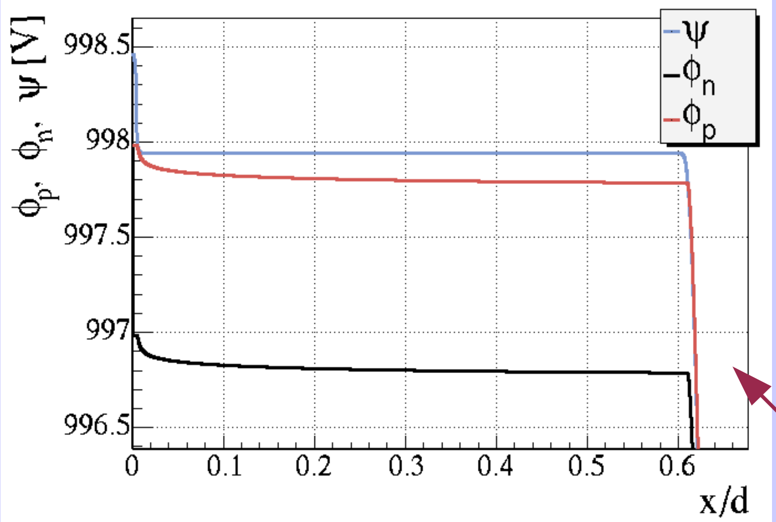
Korekcija ψ

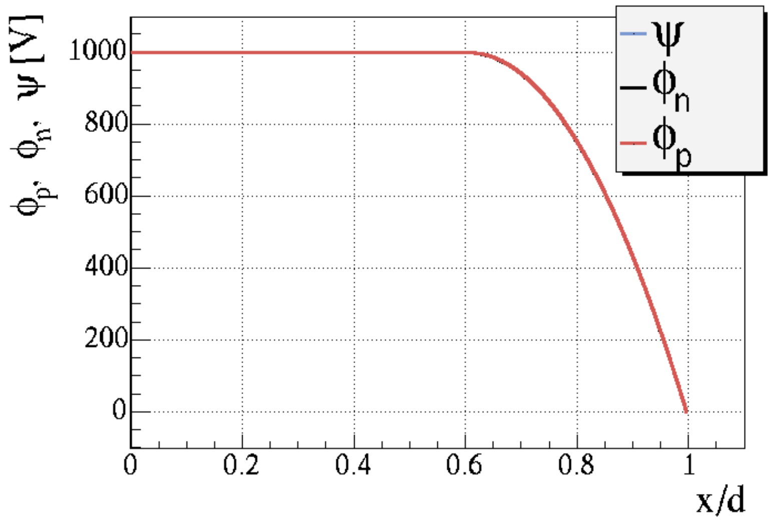


ψ po streljanju

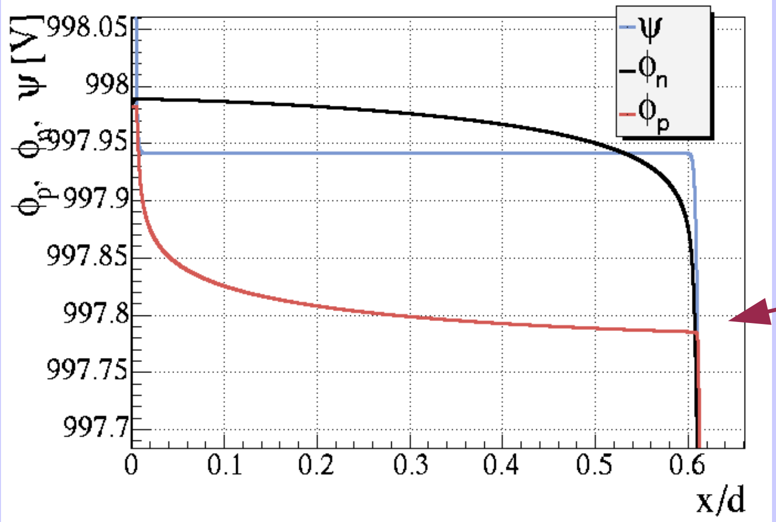
popravljen ψ

Korekcija φ_n



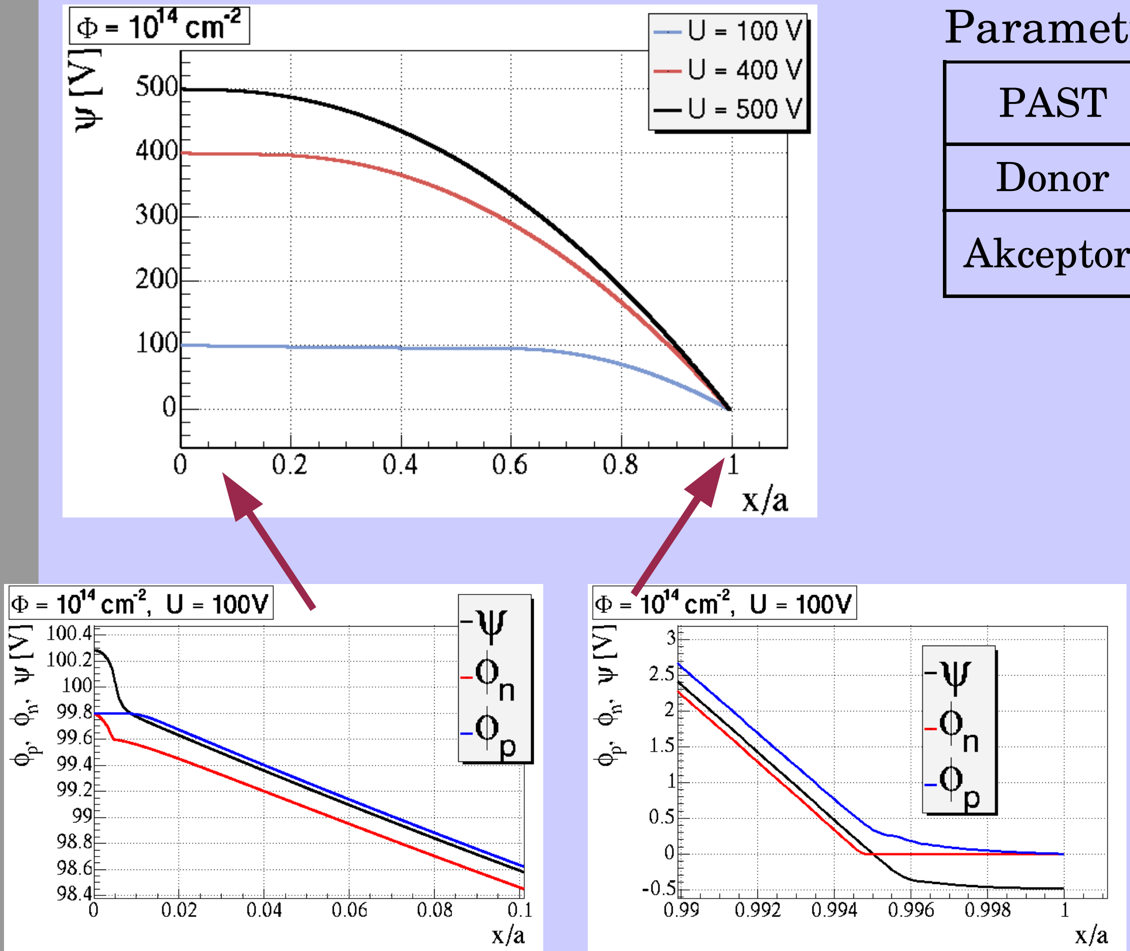


popravljen
φ_n in φ_p



φ_n in φ_p po
integraciji

Rezultati: $\Phi=1\ 10^{14}\ cm^{-2}$



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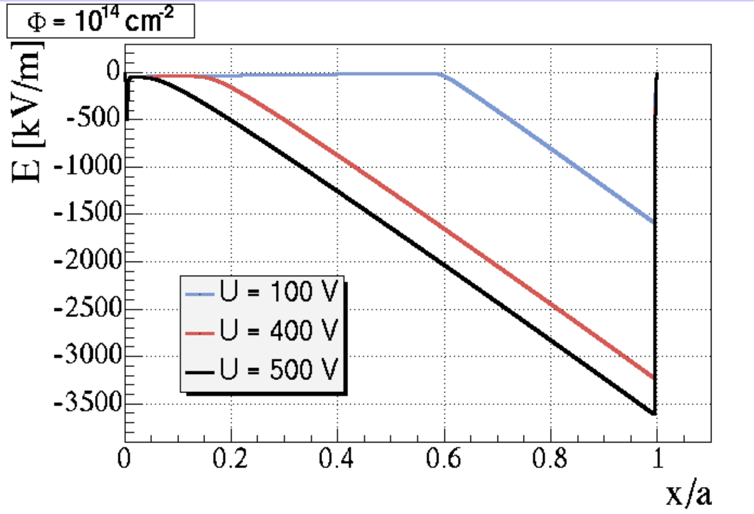
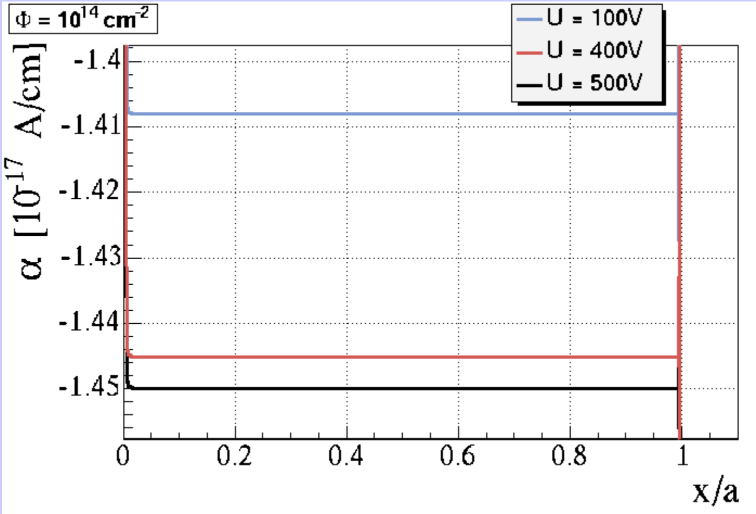
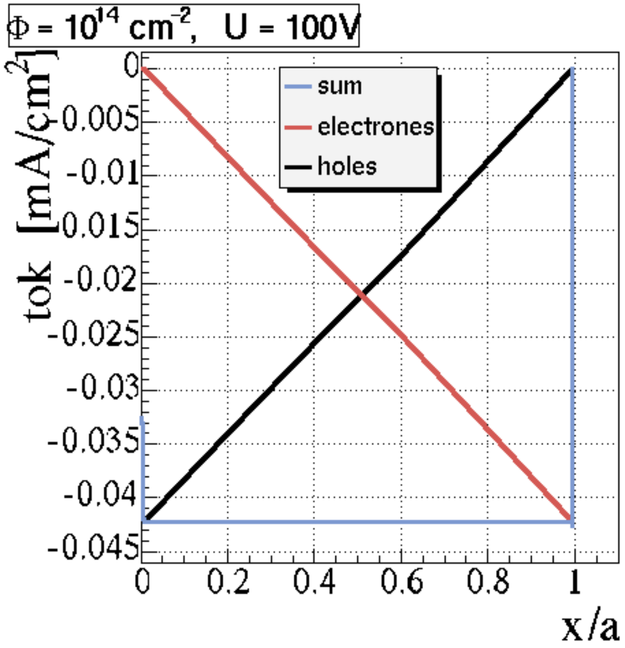
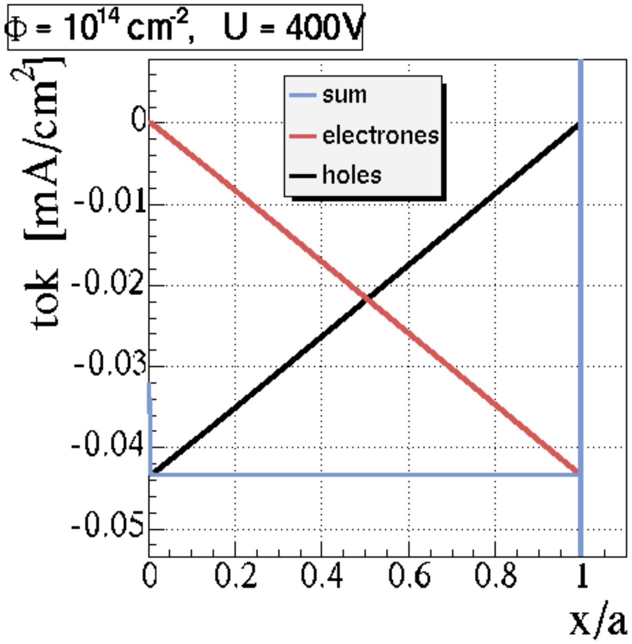
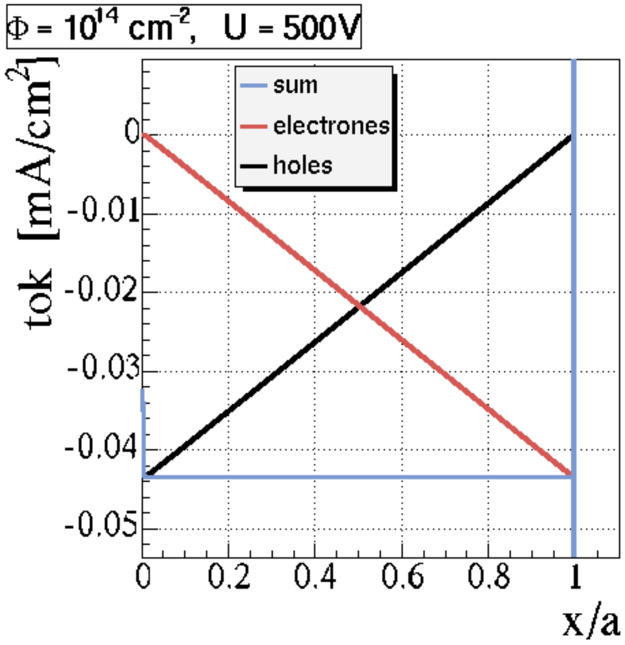




Rezultati: Φ=1 10^{14} cm^{-2}







Rezultati: $\Phi=1\ 10^{14}\ cm^{-2}$