

Aplikační příklad I

Apl. příklad 1: Izotermní vnitřní difuze v porézním katalyzátoru je popsána diferenciální rovnicí

$$y'' + \frac{a}{x} y' = \phi^2 y^n \text{ s okrajovou podmínkou } y'(0)=0 \text{ a } y(1)=1.$$

Parametr a charakterizuje tvar částice katalyzátoru $a=0$ pro desku, $a=1$ pro váleček, $a=2$ pro kuličku, n je řád reakce a ϕ Thieleho modul.

- a) Vyřešte tuto rovnici metodou sítí pro $n=0$, $a=1$ a $\phi=1$
- b) Vyřešte tuto rovnici metodou sítí pro $n=1$, $a=2$ a $\phi=1;2;4$
- c) Vyřešte tuto rovnici metodou sítí pro $n=1$, $a=0$ a $\phi=1;2;4$

a)

$n=0$, $a=1$ a $\phi=1$

```
n = 0;
```

```
aa = 1;
```

```
 $\phi$  = 1;
```

```
f[x_, y1_, y2_] =  $\phi^2$  y1n - aa / x * y2;
```

```
a = 0.0;
```

```
b = 1.0;
```

```
 $\alpha$ 1 = 0;
```

```
 $\alpha$ 2 = 1;
```

```
 $\beta$ 1 = 1;
```

```
 $\beta$ 2 = 0;
```

```
 $\gamma$ 1 = 0;
```

```
 $\gamma$ 2 = 1;
```

```
 $\epsilon$  = 0.00000001;
```

```
nn = 20;
```

```
y0 = Table[0.5, {i, 1, nn + 1}];
```

```
y0[[1]] = 1.0;
```

```
y0[[nn + 1]] = 1.0;
```

```
yres = DESite2[nn, f, a, b,  $\alpha$ 1,  $\alpha$ 2,  $\beta$ 1,  $\beta$ 2,  $\gamma$ 1,  $\gamma$ 2,  $\epsilon$ , y0, 10];
```

```
iterace = 0
```

```
y={0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5,  
0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 1.}
```

```
iterace = 1      s = 0.611237
```

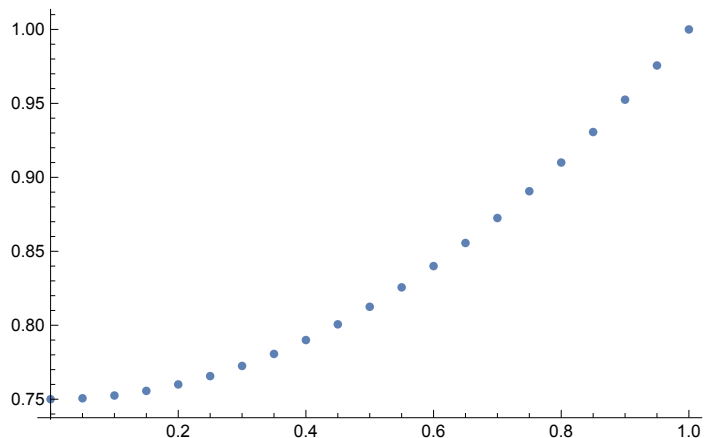
```
y={0.75, 0.750625, 0.7525, 0.755625, 0.76, 0.765625, 0.7725, 0.780625, 0.79, 0.800625, 0.8125,  
0.825625, 0.84, 0.855625, 0.8725, 0.890625, 0.91, 0.930625, 0.9525, 0.975625, 1.}
```

```
iterace = 2      s = 2.90343×10-15
```

```
y={0.75, 0.750625, 0.7525, 0.755625, 0.76, 0.765625, 0.7725, 0.780625, 0.79, 0.800625, 0.8125,
  0.825625, 0.84, 0.855625, 0.8725, 0.890625, 0.91, 0.930625, 0.9525, 0.975625, 1.}
```

Graf řešení $y_1(x)$

```
ListPlot[yres]
```

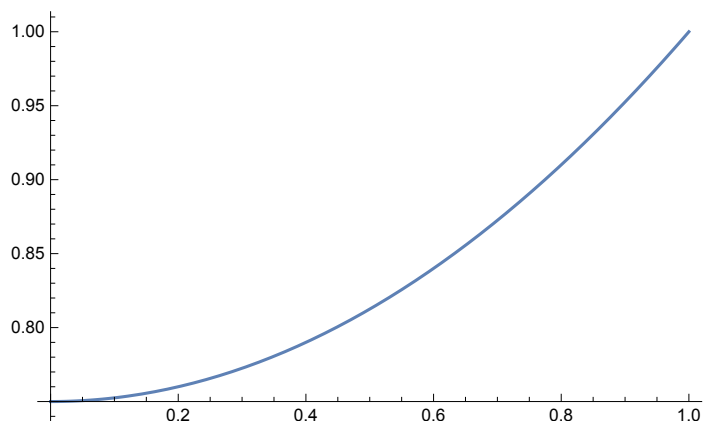


Přesné řešení

```
pres = DSolve[{y''[x] == -y'[x]/x + 1, y'[0] == 0, y[1] == 1}, y[x], x]
```

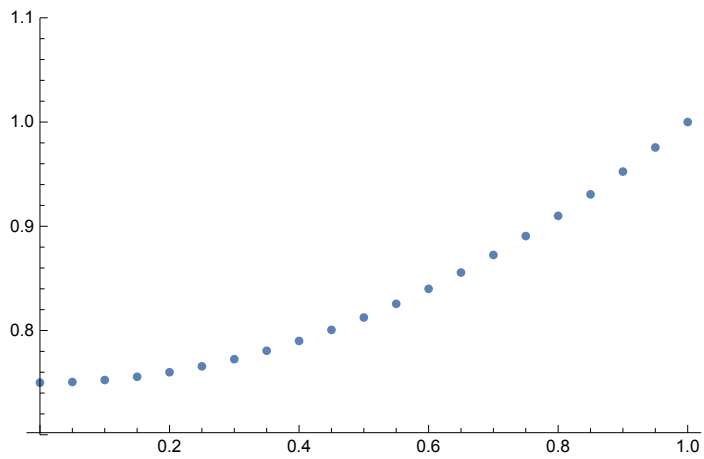
```
{ {y[x] -> 1/4 (3 + x^2)} }
```

```
gp = Plot[y[x] /. pres, {x, 0, 1}]
```

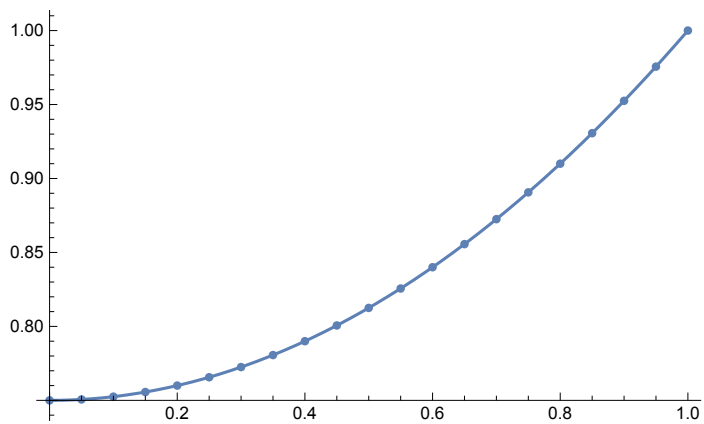


Graf řešení $y(x)$

```
g1 = ListPlot[yres, PlotRange -> {0.7, 1.1}]
```



Show[gp, g1]



Tabulka řešení $y_2(x)$

MatrixForm[yres]

0.	0.75
0.05	0.750625
0.1	0.7525
0.15	0.755625
0.2	0.76
0.25	0.765625
0.3	0.7725
0.35	0.780625
0.4	0.79
0.45	0.800625
0.5	0.8125
0.55	0.825625
0.6	0.84
0.65	0.855625
0.7	0.8725
0.75	0.890625
0.8	0.91
0.85	0.930625
0.9	0.9525
0.95	0.975625
1.	1.

b)

$n=1$, $a=2$ a $\phi=1$

$n = 1;$

$aa = 2;$

$\phi = 1;$

$f[x_, y_, dy_] = \phi^2 y^n - aa / x * dy$

$-\frac{2 dy}{x} + y$

$a = 0.0;$

$b = 1.0;$

$\alpha_1 = 0;$

$\alpha_2 = 1;$

$\beta_1 = 1;$

$\beta_2 = 0;$

$\gamma_1 = 0;$

$\gamma_2 = 1;$

$\epsilon = 0.000001;$

$nn = 20;$

$y0 = \text{Table}[0.8, \{i, 1, nn + 1\}];$

$y0[[1]] = 1.0;$

$y0[[nn + 1]] = 1.0;$

$yres = \text{DESite2}[nn, f, a, b, \alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1, \gamma_2, \epsilon, y0, 10];$

iterace = 0

$y = \{0.8, 1.\}$

iterace = 1 $s = 0.126082$

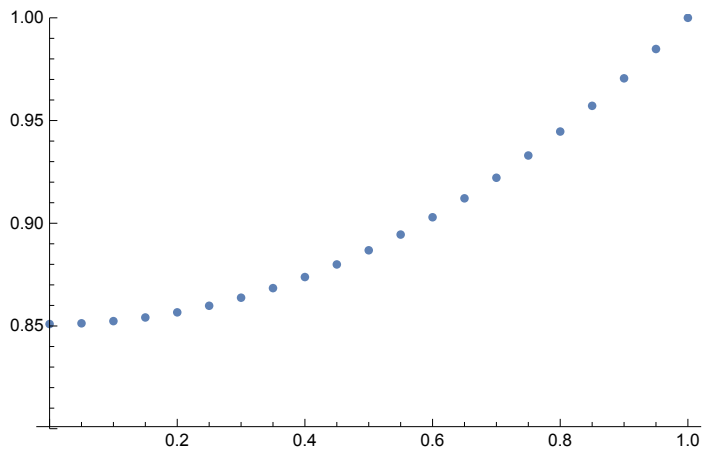
$y = \{0.850946, 0.8513, 0.852365, 0.85414, 0.856629, 0.859836, 0.863765, 0.868422, 0.873815, 0.879951, 0.88684, 0.894492, 0.902919, 0.912132, 0.922147, 0.932978, 0.944643, 0.957157, 0.970541, 0.984815, 1.\}$

iterace = 2 $s = 4.27998 \times 10^{-16}$

$y = \{0.850946, 0.8513, 0.852365, 0.85414, 0.856629, 0.859836, 0.863765, 0.868422, 0.873815, 0.879951, 0.88684, 0.894492, 0.902919, 0.912132, 0.922147, 0.932978, 0.944643, 0.957157, 0.970541, 0.984815, 1.\}$

Graf řešení $y(x)$

$g1 = \text{ListPlot}[yres, \text{PlotRange} \rightarrow \{0.8, 1\}]$



Tabulka řešení $y(x)$

MatrixForm[yres]

```
( 0.  0.850946
 0.05 0.8513
 0.1  0.852365
 0.15 0.85414
 0.2  0.856629
 0.25 0.859836
 0.3  0.863765
 0.35 0.868422
 0.4  0.873815
 0.45 0.879951
 0.5  0.88684
 0.55 0.894492
 0.6  0.902919
 0.65 0.912132
 0.7  0.922147
 0.75 0.932978
 0.8  0.944643
 0.85 0.957157
 0.9  0.970541
 0.95 0.984815
 1.  1.)
```

$n=1$, $a=2$ a $\phi=2$

```
n = 1;
aa = 2;
phi = 2;
```

```
f[x_, y_, dy_] = phi^2 y^n - aa / x * dy
```

```
- 2 dy / x + 4 y
```

```

a = 0.0;
b = 1.0;
 $\alpha_1$  = 0;
 $\alpha_2$  = 1;
 $\beta_1$  = 1;
 $\beta_2$  = 0;
 $\gamma_1$  = 0;
 $\gamma_2$  = 1;
 $\epsilon$  = 0.000001;
nn = 20;
y0 = Table[0.8, {i, 1, nn + 1}];
y0[[1]] = 1.0;
y0[[nn + 1]] = 1.0;

yres = DESite2[nn, f, a, b,  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$ ,  $\beta_2$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\epsilon$ , y0, 10];

iterace = 0

y={0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8,
  0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 1.}

iterace = 1      s = 0.207337

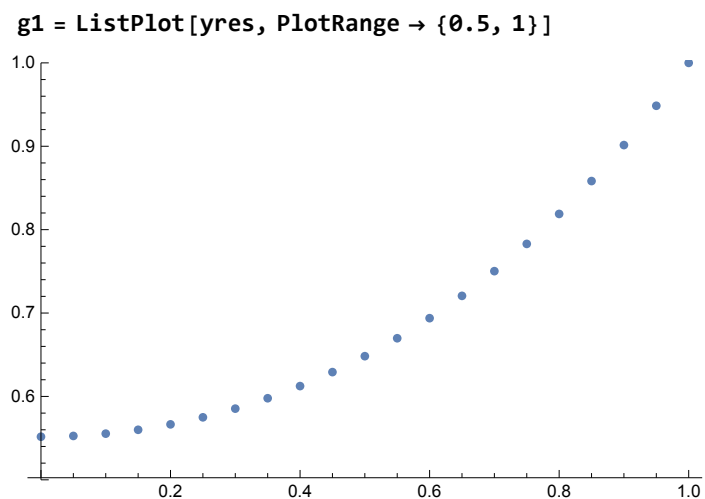
y={0.551686, 0.552607, 0.55537, 0.559993, 0.566505, 0.574944,
  0.585361, 0.59782, 0.612394, 0.629174, 0.64826, 0.669769, 0.693833,
  0.720599, 0.750233, 0.782918, 0.818857, 0.858274, 0.901418, 0.948561, 1.}

iterace = 2      s = 1.69367  $\times 10^{-15}$ 

y={0.551686, 0.552607, 0.55537, 0.559993, 0.566505, 0.574944,
  0.585361, 0.59782, 0.612394, 0.629174, 0.64826, 0.669769, 0.693833,
  0.720599, 0.750233, 0.782918, 0.818857, 0.858274, 0.901418, 0.948561, 1.}

```

Graf řešení $y(x)$



Tabulka řešení $y(x)$

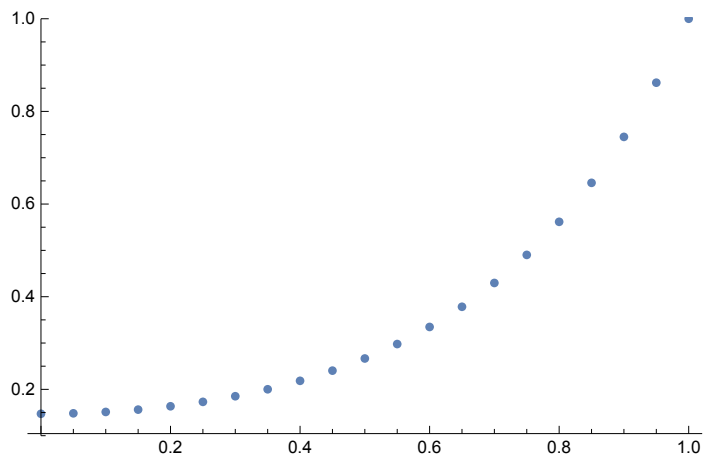
```
MatrixForm[yres]
```



```
y={0.147298, 0.148287, 0.151253, 0.156275, 0.163474, 0.173025,
  0.185159, 0.200175, 0.218443, 0.240418, 0.266654, 0.297816, 0.334704,
  0.378275, 0.429672, 0.490257, 0.561654, 0.645795, 0.744985, 0.861964, 1.}
```

Graf řešení $y(x)$

```
g1 = ListPlot[yres, PlotRange -> {0.1, 1}]
```



Tabulka řešení $y(x)$

```
MatrixForm[yres]
```

$$\begin{pmatrix} 0. & 0.147298 \\ 0.05 & 0.148287 \\ 0.1 & 0.151253 \\ 0.15 & 0.156275 \\ 0.2 & 0.163474 \\ 0.25 & 0.173025 \\ 0.3 & 0.185159 \\ 0.35 & 0.200175 \\ 0.4 & 0.218443 \\ 0.45 & 0.240418 \\ 0.5 & 0.266654 \\ 0.55 & 0.297816 \\ 0.6 & 0.334704 \\ 0.65 & 0.378275 \\ 0.7 & 0.429672 \\ 0.75 & 0.490257 \\ 0.8 & 0.561654 \\ 0.85 & 0.645795 \\ 0.9 & 0.744985 \\ 0.95 & 0.861964 \\ 1. & 1. \end{pmatrix}$$

c)

$n=1$, $a=0$ a $\phi=1$

```
n = 1;
aa = 0;
phi = 1;
```

```
f[x_, y_, dy_] =  $\phi^2 y^n$  - aa / x * dy
```

```
y
```

```
a = 0.0;
b = 1.0;
 $\alpha_1$  = 0;
 $\alpha_2$  = 1;
 $\beta_1$  = 1;
 $\beta_2$  = 0;
 $\gamma_1$  = 0;
 $\gamma_2$  = 1;
 $\epsilon$  = 0.000001;
nn = 20;
y0 = Table[0.8, {i, 1, nn + 1}];
y0[[1]] = 1.0;
y0[[nn + 1]] = 1.0;

yres = DESite2[nn, f, a, b,  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$ ,  $\beta_2$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\epsilon$ , y0, 10];

iterace = 0

y={0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8,
  0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 1.}

iterace = 1      s = 0.131157

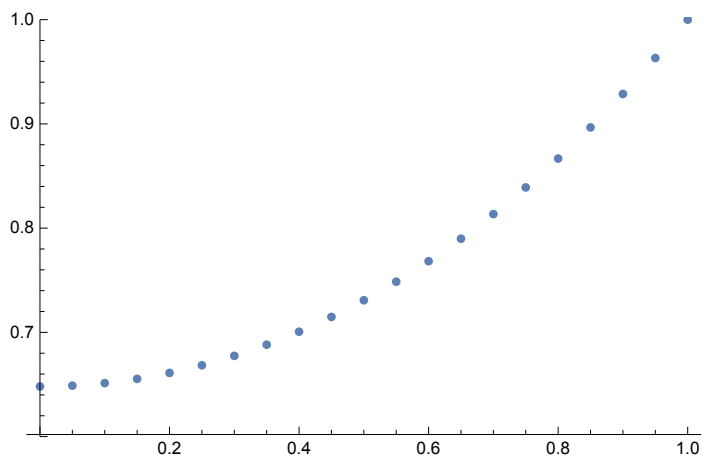
y={0.64809, 0.648901, 0.651335, 0.655396, 0.661097, 0.66845,
  0.677474, 0.688191, 0.70063, 0.714819, 0.730796, 0.7486, 0.768276,
  0.789872, 0.813442, 0.839047, 0.866749, 0.896617, 0.928728, 0.96316, 1.}

iterace = 2      s = 5.89213  $\times 10^{-16}$ 

y={0.64809, 0.648901, 0.651335, 0.655396, 0.661097, 0.66845,
  0.677474, 0.688191, 0.70063, 0.714819, 0.730796, 0.7486, 0.768276,
  0.789872, 0.813442, 0.839047, 0.866749, 0.896617, 0.928728, 0.96316, 1.}
```

Graf řešení $y(x)$

```
g1 = ListPlot[yres, PlotRange -> {0.6, 1}]
```



Tabulka řešení $y(x)$

MatrixForm[yres]

$$\begin{pmatrix} 0. & 0.64809 \\ 0.05 & 0.648901 \\ 0.1 & 0.651335 \\ 0.15 & 0.655396 \\ 0.2 & 0.661097 \\ 0.25 & 0.66845 \\ 0.3 & 0.677474 \\ 0.35 & 0.688191 \\ 0.4 & 0.70063 \\ 0.45 & 0.714819 \\ 0.5 & 0.730796 \\ 0.55 & 0.7486 \\ 0.6 & 0.768276 \\ 0.65 & 0.789872 \\ 0.7 & 0.813442 \\ 0.75 & 0.839047 \\ 0.8 & 0.866749 \\ 0.85 & 0.896617 \\ 0.9 & 0.928728 \\ 0.95 & 0.96316 \\ 1. & 1. \end{pmatrix}$$

n=1, a=0 a $\phi=2$

n = 1;

aa = 0;

$\phi = 2$;

f[x_, y_, dy_] = $\phi^2 y^n - aa / x * dy$

4 y

a = 0.0;

b = 1.0;

$\alpha_1 = 0$;

$\alpha_2 = 1$;

$\beta_1 = 1$;

$\beta_2 = 0$;

$\gamma_1 = 0$;

$\gamma_2 = 1$;

$\epsilon = 0.000001$;

nn = 20;

y0 = Table[0.8, {i, 1, nn + 1}];

y0[[1]] = 1.0;

y0[[nn + 1]] = 1.0;

yres = DESite2[nn, f, a, b, α_1 , α_2 , β_1 , β_2 , γ_1 , γ_2 , ϵ , y0, 10];

iterace = 0

**y={0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8,
0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 1.}**

iterace = 1 s = 0.468255

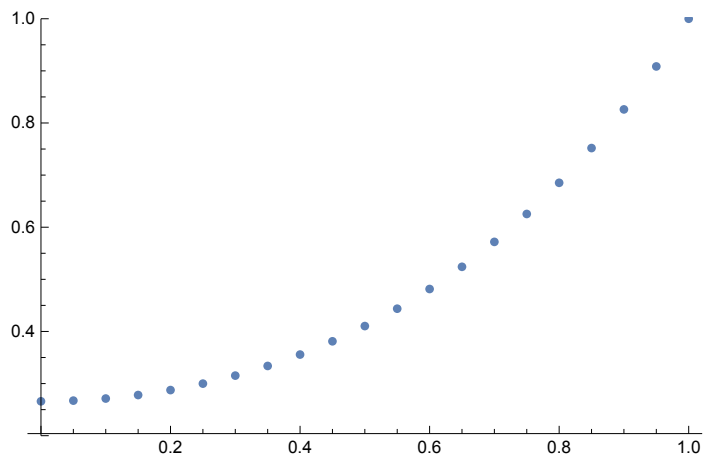
**y={0.265951, 0.267288, 0.271297, 0.278019, 0.287522, 0.299899,
0.315276, 0.333806, 0.355673, 0.381097, 0.410333, 0.443671, 0.481446,
0.524036, 0.571866, 0.625415, 0.685218, 0.751873, 0.826047, 0.908481, 1.}**

iterace = 2 s = 1.01445×10^{-14}

```
y={0.265951, 0.267288, 0.271297, 0.278019, 0.287522, 0.299899,
  0.315276, 0.333806, 0.355673, 0.381097, 0.410333, 0.443671, 0.481446,
  0.524036, 0.571866, 0.625415, 0.685218, 0.751873, 0.826047, 0.908481, 1.}
```

Graf řešení $y(x)$

```
g1 = ListPlot[yres, PlotRange -> {0.2, 1}]
```



Tabulka řešení $y(x)$

```
MatrixForm[yres]
```

$$\begin{pmatrix} 0. & 0.265951 \\ 0.05 & 0.267288 \\ 0.1 & 0.271297 \\ 0.15 & 0.278019 \\ 0.2 & 0.287522 \\ 0.25 & 0.299899 \\ 0.3 & 0.315276 \\ 0.35 & 0.333806 \\ 0.4 & 0.355673 \\ 0.45 & 0.381097 \\ 0.5 & 0.410333 \\ 0.55 & 0.443671 \\ 0.6 & 0.481446 \\ 0.65 & 0.524036 \\ 0.7 & 0.571866 \\ 0.75 & 0.625415 \\ 0.8 & 0.685218 \\ 0.85 & 0.751873 \\ 0.9 & 0.826047 \\ 0.95 & 0.908481 \\ 1. & 1. \end{pmatrix}$$

$n=1$, $a=0$ a $\phi=4$

```
n = 1;
```

```
aa = 0;
```

```
 $\phi = 4$ ;
```

```
f[x_, y_, dy_] =  $\phi^2 y^n$  - aa / x * dy
```

16 y

```

a = 0.0;
b = 1.0;
 $\alpha_1$  = 0;
 $\alpha_2$  = 1;
 $\beta_1$  = 1;
 $\beta_2$  = 0;
 $\gamma_1$  = 0;
 $\gamma_2$  = 1;
 $\epsilon$  = 0.000001;
nn = 20;
y0 = Table[0.8, {i, 1, nn + 1}];
y0[[1]] = 1.0;
y0[[nn + 1]] = 1.0;

yres = DESite2[nn, f, a, b,  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$ ,  $\beta_2$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\epsilon$ , y0, 10];

iterace = 0

y={0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8,
  0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 1.}

iterace = 1      s = 0.741451

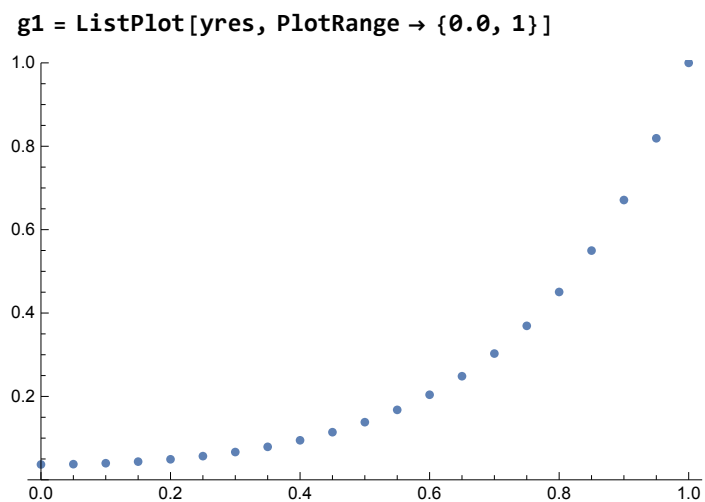
y={0.036788, 0.0375388, 0.0397911, 0.0436351, 0.0492245, 0.0567828,
  0.0666125, 0.0791067, 0.0947651, 0.114214, 0.138232, 0.167779, 0.204037,
  0.248456, 0.302814, 0.369284, 0.450526, 0.549788, 0.671043, 0.819139, 1.}

iterace = 2      s = 1.30413  $\times 10^{-15}$ 

y={0.036788, 0.0375388, 0.0397911, 0.0436351, 0.0492245, 0.0567828,
  0.0666125, 0.0791067, 0.0947651, 0.114214, 0.138232, 0.167779, 0.204037,
  0.248456, 0.302814, 0.369284, 0.450526, 0.549788, 0.671043, 0.819139, 1.}

```

Graf řešení $y(x)$



Tabulka řešení $y(x)$

```
MatrixForm[yres]
```

$$\begin{pmatrix} 0. & 0.036788 \\ 0.05 & 0.0375388 \\ 0.1 & 0.0397911 \\ 0.15 & 0.0436351 \\ 0.2 & 0.0492245 \\ 0.25 & 0.0567828 \\ 0.3 & 0.0666125 \\ 0.35 & 0.0791067 \\ 0.4 & 0.0947651 \\ 0.45 & 0.114214 \\ 0.5 & 0.138232 \\ 0.55 & 0.167779 \\ 0.6 & 0.204037 \\ 0.65 & 0.248456 \\ 0.7 & 0.302814 \\ 0.75 & 0.369284 \\ 0.8 & 0.450526 \\ 0.85 & 0.549788 \\ 0.9 & 0.671043 \\ 0.95 & 0.819139 \\ 1. & 1. \end{pmatrix}$$