

```
[> read "DESite.m":
```

Apl. p íklad 1:

Izotermní vnit ní difuze v porézním katalyzátoru je popsána diferenciální rovnicí

$y'' + a/x y' = \phi^2 y^n$ s okrajovou podmínkou $y'(0)=0$ 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 Thieleho modul.

a) Vyřešte tuto rovnici metodou sítí pro $n=0$, $a=1$ a $a=2$

b) Vyřešte tuto rovnici metodou sítí pro $n=1$, $a=2$ a $a=1;2;4$

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

a)

Definice parametrů diferenciální rovnice

Lineární rovnice

```
> n1:=0:  
aa:=1:  
phi:=1:
```

Definice pravé strany diferenciální rovnice

```
> f:=(x,y,dy)->-aa/x*dy + phi^2*y^n1 ;
```

$$f := (x, y, dy) \rightarrow -\frac{aa}{x} \frac{dy}{dx} + \phi^2 y^{n1} \quad (1.1)$$

Definice parametrů metody

```
> a := 0:  
b := 1:  
alfa1 := 0:  
alfa2 := 1:  
beta1 := 1:  
beta2 := 0:  
gama1 := 0:  
gama2 := 1:  
eps := 0.1e-3:  
n := 20:  
y0:=evalf([seq(0.5,i=1..n+1)]);  
y0[1]:=1.0;  
y0[n+1]:=1.0;
```

```
y0 := [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, 0.5,  
0.5, 0.5]
```

```
y0_1 := 1.0
```

```
y0_21 := 1.0
```

(1.2)

```
> yres := DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,  
gama2, eps, y0, 10):
```

```
"iterace = ", 0
```

```
"y = ", [0.5000000000, 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, 0.5, 0.5, 0.5, 1.]
```

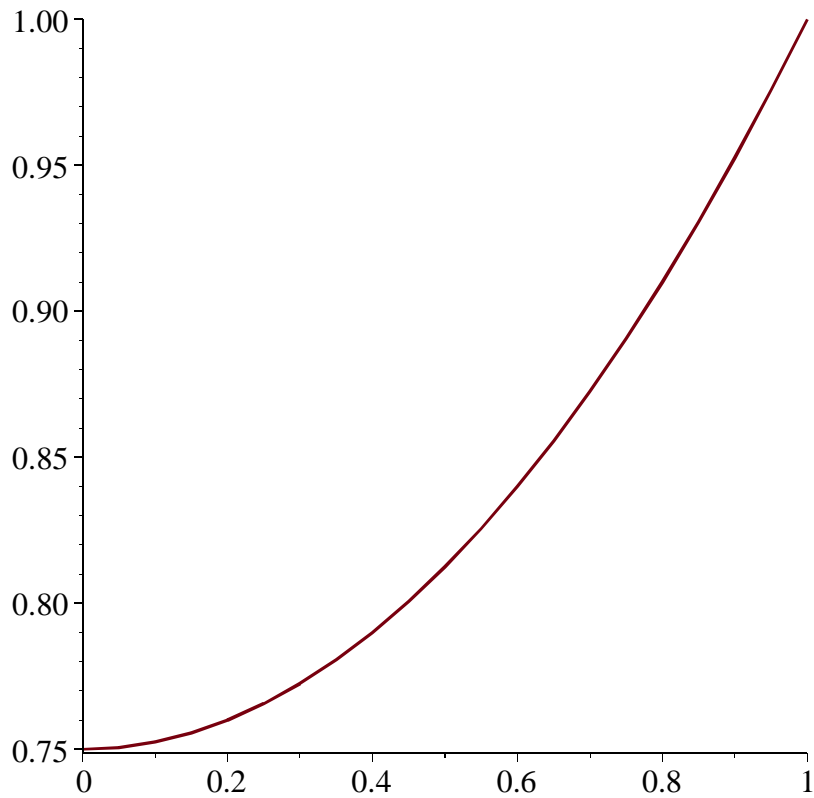
```
"iterace = ", 1, " s = ", 0.6112373246
```

```
"y = ", [0.7499999999, 0.7506249997, 0.7524999997, 0.7556249997, 0.7599999997,  
0.7656249997, 0.7724999997, 0.7806249997, 0.7899999997, 0.8006249997,  
0.8124999997, 0.8256249997, 0.8399999997, 0.8556249997, 0.8724999997,  
0.8906249997, 0.9099999997, 0.9306249997, 0.9524999997, 0.9756249997, 1.]
```

```
"iterace = ", 2, "    s = ", 3.501912068 10-8  
"y = ", [0.7500000399, 0.7506250397, 0.7525000395, 0.7556250390, 0.7600000383,  
0.7656250374, 0.7725000363, 0.7806250350, 0.7900000335, 0.8006250319,  
0.8125000300, 0.8256250279, 0.8400000256, 0.8556250231, 0.8725000204,  
0.8906250175, 0.9100000144, 0.9306250111, 0.9525000076, 0.9756250039, 1.]
```

(1.3)

```
> # Graf funkce yres(x)  
> plot(yres);
```



```
> # Tabulka hodnot funkce y(x)  
> linalg[matrix](yres);
```

0.	0.7500000399
0.05000000000	0.7506250397
0.1000000000	0.7525000395
0.1500000000	0.7556250390
0.2000000000	0.7600000383
0.2500000000	0.7656250374
0.3000000000	0.7725000363
0.3500000000	0.7806250350
0.4000000000	0.7900000335
0.4500000000	0.8006250319
0.5000000000	0.8125000300
0.5500000000	0.8256250279
0.6000000000	0.8400000256
0.6500000000	0.8556250231
0.7000000000	0.8725000204
0.7500000000	0.8906250175
0.8000000000	0.9100000144
0.8500000000	0.9306250111
0.9000000000	0.9525000076
0.9500000000	0.9756250039
1.0000000000	1.

(1.4)

b)

Definice parametrů diferenciální rovnice

```
> n1:=1:
  aa:=2:
  phi:=1:
```

Definice pravé strany diferenciální rovnice

```
> f:=(x,y,dy)->-aa/x*dy + phi^2*y^n1 ;
```

$$f := (x, y, dy) \rightarrow -\frac{aa \, dy}{x} + \phi^2 y^{n1}$$

(2.1)

Definice parametrů metody

```
> a := 0:
  b := 1:
  alfa1 := 0:
  alfa2 := 1:
  beta1 := 1:
  beta2 := 0:
  gama1 := 0:
  gama2 := 1:
  eps := 0.1e-5:
  n := 20:
```

```

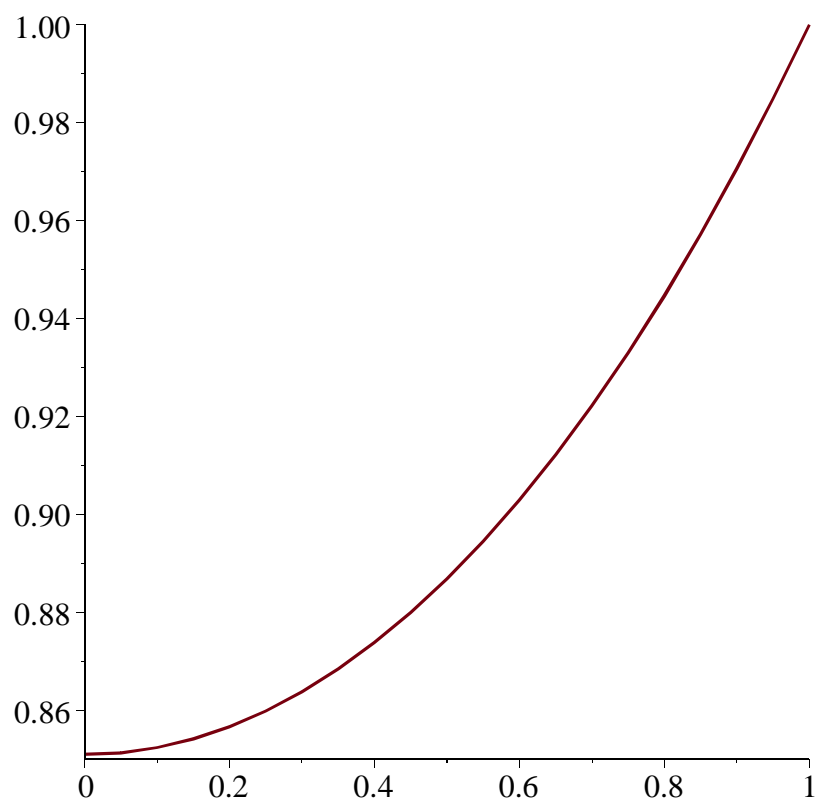
y0:=evalf([seq(0.8,i=1..n+1)]);
y0[1]:=1.0;
y0[n+1]:=1.0;
y0:=[0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8,0.8]

y01 := 1.0
y021 := 1.0
(2.2)

> yres := DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,
gama2, eps, y0, 10):
"iterace = ", 0
"y = ", [0.7999999999, 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, 0.8, 1.]
"iterace = ", 1, " s = ", 0.1260824218
"y = ", [0.8509456896, 0.8513003979, 0.8523645234, 0.8541398394, 0.8566290097, 0.8598357698, 0.8637649344, 0.8684224054, 0.8738151826, 0.8799513763, 0.8868402219, 0.8944920961, 0.9029185356, 0.9121322581, 0.9221471843, 0.9329784638, 0.9446425016, 0.9571569879, 0.9705409298, 0.9848146852, 1.]
"iterace = ", 2, " s = ", 4.234082026 10-9
"y = ", [0.8509456839, 0.8513003924, 0.8523645180, 0.8541398342, 0.8566290046, 0.8598357646, 0.8637649294, 0.8684224007, 0.8738151784, 0.8799513723, 0.8868402185, 0.8944920932, 0.9029185331, 0.9121322555, 0.9221471816, 0.9329784613, 0.9446424997, 0.9571569864, 0.9705409287, 0.9848146849, 1.]
(2.3)

> # Graf funkce y(x)
> plot(yres);

```



```
> # Tabulka hodnot funkce y(x)  
> linalg[matrix](yres);
```


$$y_{0_1} := 1.0$$

$$y_{0_{21}} := 1.0$$

(2.6)

```
> yres:= DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,gama2,
eps, y0, 10):
```

```
"iterace = ", 0
```

```
"y = ", [0.7999999999, 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 = ", 0.2073367222
```

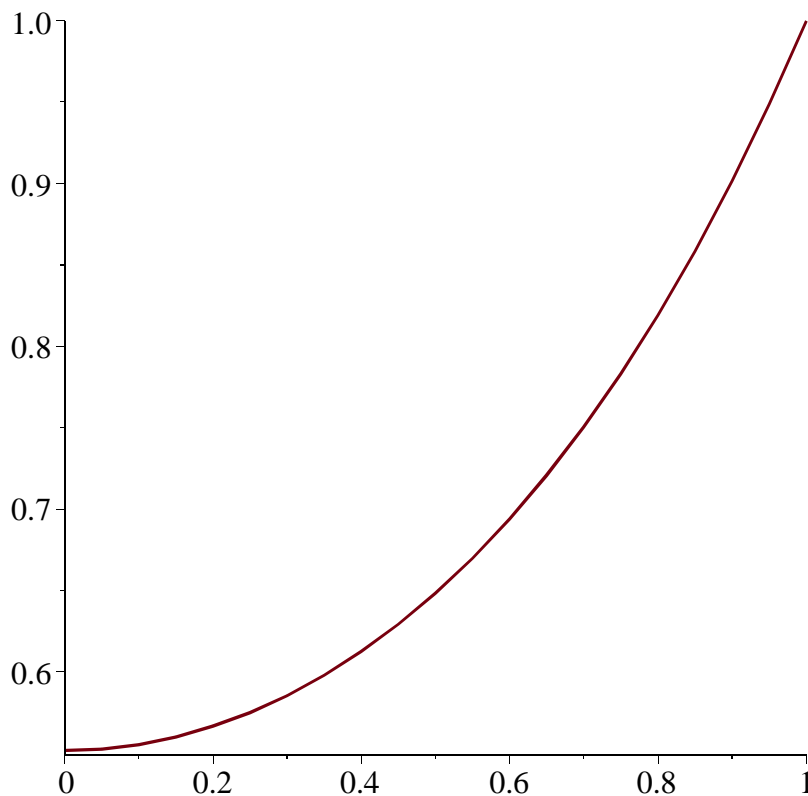
```
"y = ", [0.5516859493, 0.5526069609, 0.5553699957, 0.5599934740, 0.5665051642,
0.5749442197, 0.5853614586, 0.5978197276, 0.6123943520, 0.6291736763,
0.6482596988, 0.6697688053, 0.6938326082, 0.7205988963, 0.7502327044,
0.7829175100, 0.8188565666, 0.8582743842, 0.9014183691, 0.9485606348, 1.]
```

```
"iterace = ", 2, " s = ", 1.709763815 10-9
```

```
"y = ", [0.5516859509, 0.5526069627, 0.5553699977, 0.5599934757, 0.5665051658,
0.5749442208, 0.5853614590, 0.5978197272, 0.6123943508, 0.6291736745,
0.6482596969, 0.6697688037, 0.6938326071, 0.7205988953, 0.7502327038,
0.7829175099, 0.8188565669, 0.8582743848, 0.9014183694, 0.9485606348, 1.]
```

(2.7)

```
> plot(yres);
```



```
> linalg[matrix](yres);
```


$$y_{0_1} := 1.0$$

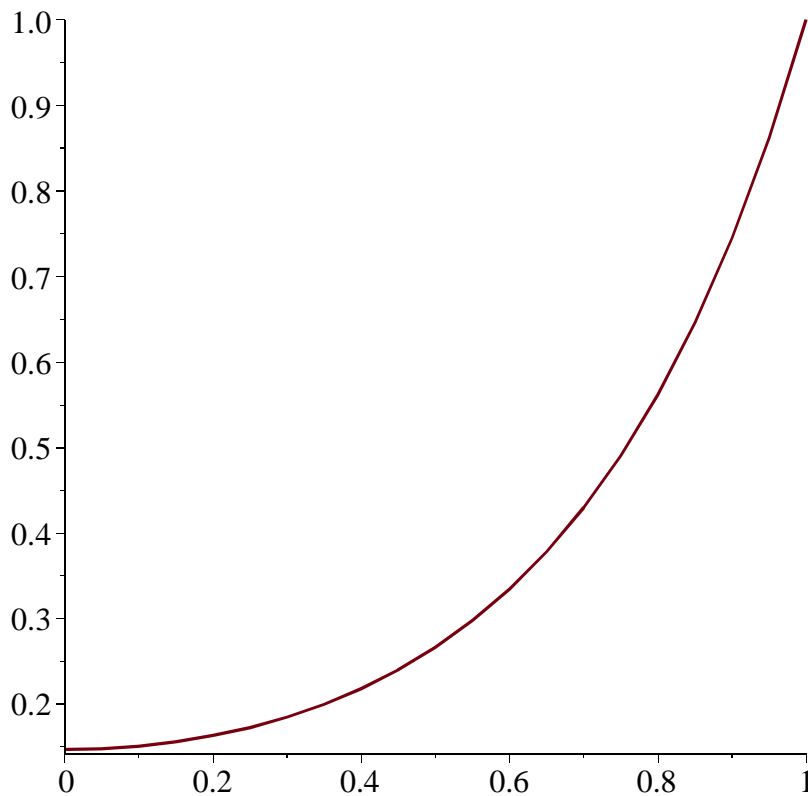
$$y_{0_{21}} := 1.0$$

(2.10)

```
> yres := DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,
  gama2, eps, y0, 10):
  "iterace = ", 0
"y = ", [0.7999999999, 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 = ", 0.6094049063
"y = ", [0.1472983089, 0.1482868882, 0.1512526260, 0.1562746084, 0.1634738378,
  0.1730245383, 0.1851591565, 0.2001750552, 0.2184431062, 0.2404184564,
  0.2666538008, 0.2978155843, 0.3347036422, 0.3782749025, 0.4296719079,
  0.4902570638, 0.5616537150, 0.6457953708, 0.7449846678, 0.8619639840, 1.]
  "iterace = ", 2, "    s = ", 8.689880451 10-10
"y = ", [0.1472983089, 0.1482868882, 0.1512526260, 0.1562746086, 0.1634738382,
  0.1730245387, 0.1851591571, 0.2001750555, 0.2184431063, 0.2404184563,
  0.2666538007, 0.2978155843, 0.3347036421, 0.3782749024, 0.4296719076,
  0.4902570633, 0.5616537144, 0.6457953699, 0.7449846670, 0.8619639836, 1.]
```

(2.11)

```
> plot(yres);
```



```
> linalg[matrix](yres);
```

0.	0.1472983089
0.05000000000	0.1482868882
0.1000000000	0.1512526260
0.1500000000	0.1562746086
0.2000000000	0.1634738382
0.2500000000	0.1730245387
0.3000000000	0.1851591571
0.3500000000	0.2001750555
0.4000000000	0.2184431063
0.4500000000	0.2404184563
0.5000000000	0.2666538007
0.5500000000	0.2978155843
0.6000000000	0.3347036421
0.6500000000	0.3782749024
0.7000000000	0.4296719076
0.7500000000	0.4902570633
0.8000000000	0.5616537144
0.8500000000	0.6457953699
0.9000000000	0.7449846670
0.9500000000	0.8619639836
1.0000000000	1.

(2.12)

c)

Definice parametrů diferenciální rovnice

```
> n1:=1:
  aa:=0:
  phi:=1:
```

Definice pravé strany diferenciální rovnice

```
> f:=(x,y,dy)->-aa/x*dy + phi^2*y^n1 ;
```

$$f := (x, y, dy) \rightarrow -\frac{aa}{x} \frac{dy}{dx} + \phi^2 y^{n1}$$

(3.1)

Definice parametrů metody

```
> a := 0:
  b := 1:
  alfa1 := 0:
  alfa2 := 1:
  beta1 := 1:
  beta2 := 0:
  gama1 := 0:
  gama2 := 1:
  eps := 0.1e-5:
  n := 20:
  y0:=evalf([seq(0.8,i=1..n+1)]);
  y0[1]:=1.0;
```

```

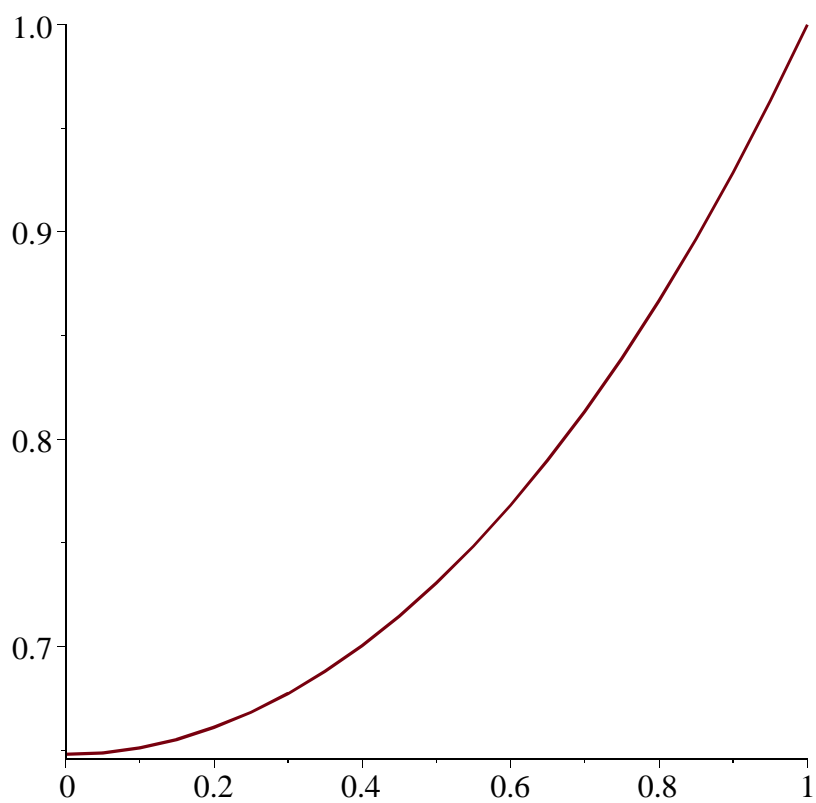
y0[n+1]:=1.0;
y0 := [0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8, 0.8,
0.8, 0.8]

y01 := 1.0
y021 := 1.0 (3.2)

> yres:= DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,gama2,
eps, y0, 10):
"iterace = ", 0
"y = ", [0.7999999999, 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 = ", 0.1311571478
"y = ", [0.6480902313, 0.6489013583, 0.6513347385, 0.6553964556, 0.6610966639,
0.6684496137, 0.6774736876, 0.6881914457, 0.7006296825, 0.7148194934,
0.7307963531, 0.7486002037, 0.7682755547, 0.7898715947, 0.8134423136,
0.8390466384, 0.8667485797, 0.8966173925, 0.9287277488, 0.9631599245, 1.]
"iterace = ", 2, " s = ", 9.016820882 10-9
"y = ", [0.6480902359, 0.6489013630, 0.6513347441, 0.6553964621, 0.6610966710,
0.6684496218, 0.6774736963, 0.6881914548, 0.7006296915, 0.7148195025,
0.7307963624, 0.7486002131, 0.7682755638, 0.7898716031, 0.8134423210,
0.8390466445, 0.8667485847, 0.8966173961, 0.9287277509, 0.9631599256, 1.] (3.3)

> # Graf funkce y(x)
> plot(yres);

```



```
> # Tabulka hodnot funkce y(x)  
> linalg[matrix](yres);
```


$$y_{0_1} := 1.0$$

$$y_{0_{21}} := 1.0$$

(3.6)

```
> yres:= DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,gama2,
eps, y0, 10):
```

```
"iterace = ", 0
```

```
"y = ", [0.7999999999, 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 = ", 0.4682546864
```

```
"y = ", [0.2659512700, 0.2672877084, 0.2712970239, 0.2780193095, 0.2875217880,
0.2998994844, 0.3152761756, 0.3338056286, 0.3556731379, 0.3810973787,
0.4103325935, 0.4436711343, 0.4814463866, 0.5240361028, 0.5718661800,
0.6254149189, 0.6852178070, 0.7518728730, 0.8260466678, 0.9084809293, 1.]
```

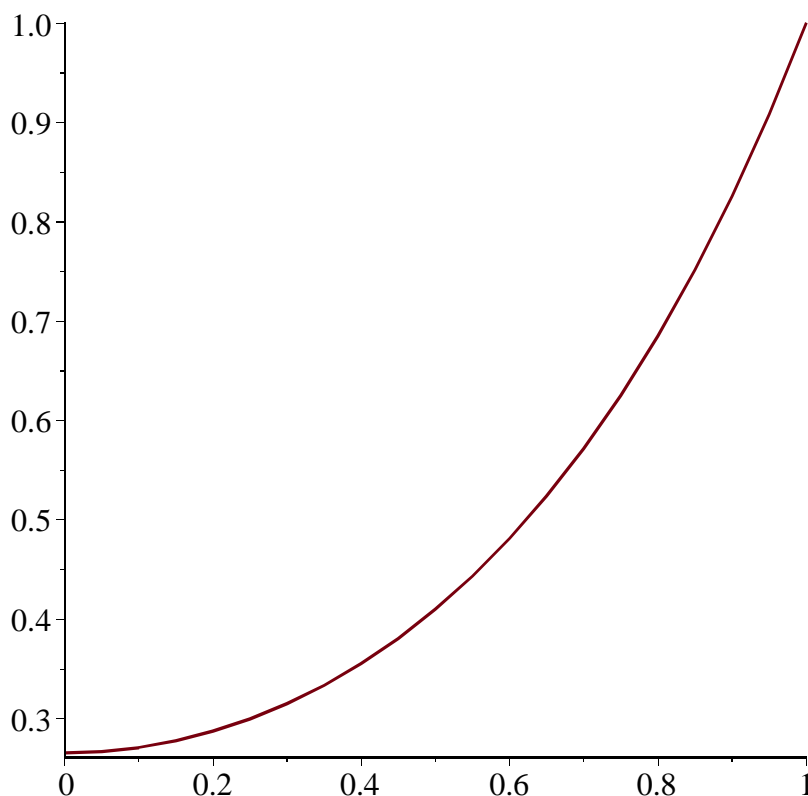
```
"iterace = ", 2, " s = ", 3.066550401 10-9
```

```
"y = ", [0.2659512680, 0.2672877065, 0.2712970219, 0.2780193076, 0.2875217863,
0.2998994830, 0.3152761744, 0.3338056276, 0.3556731370, 0.3810973779,
0.4103325925, 0.4436711330, 0.4814463849, 0.5240361006, 0.5718661777,
0.6254149166, 0.6852178048, 0.7518728711, 0.8260466662, 0.9084809282, 1.]
```

(3.7)

```
> # Graf funkce y(x)
```

```
> plot(yres);
```



```
> # Tabulka hodnot funkce y(x)
```

```
> linalg[matrix] (yres);
```

0.	0.2659512680
0.0500000000	0.2672877065
0.1000000000	0.2712970219
0.1500000000	0.2780193076
0.2000000000	0.2875217863
0.2500000000	0.2998994830
0.3000000000	0.3152761744
0.3500000000	0.3338056276
0.4000000000	0.3556731370
0.4500000000	0.3810973779
0.5000000000	0.4103325925
0.5500000000	0.4436711330
0.6000000000	0.4814463849
0.6500000000	0.5240361006
0.7000000000	0.5718661777
0.7500000000	0.6254149166
0.8000000000	0.6852178048
0.8500000000	0.7518728711
0.9000000000	0.8260466662
0.9500000000	0.9084809282
1.000000000	1.

(3.8)

Definice parametrů diferenciální rovnice

```
> n1:=1:
aa:=0:
phi:=4:
```

Definice pravé strany diferenciální rovnice

```
> f:=(x,y,dy)->-aa/x*dy + phi^2*y^n1 ;
```

$$f := (x, y, dy) \rightarrow -\frac{aa \, dy}{x} + \phi^2 y^{nl}$$

(3.9)

Definice parametrů metody

```
> a := 0:
b := 1:
alfa1 := 0:
alfa2 := 1:
beta1 := 1:
beta2 := 0:
gama1 := 0:
gama2 := 1:
eps := 0.1e-5:
n := 20:
y0:=evalf([seq(0.8,i=1..n+1)]);
y0[1]:=1.0;
y0[n+1]:=1.0;
```

[illegible]

0.8, 0.8]

$y_{0_1} := 1.0$

$y_{0_{21}} := 1.0$

(3.10)

```
> yres:= DESite2(n,f,a, b,alfa1,alfa2,beta1,beta2,gama1,gama2,
eps, y0, 10):
```

"iterace = ", 0

"y = ", [0.7999999999, 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, 0.8, 1.]

"iterace = ", 1, " s = ", 0.7414509126

"y = ", [0.03678801740, 0.0375387932, 0.0397911206, 0.0436350928, 0.0492244686, 0.0567828231, 0.0666124907, 0.0791066582, 0.0947650922, 0.1142141296, 0.1382317326, 0.1677786047, 0.2040366210, 0.2484561022, 0.3028138274, 0.3692841055, 0.4505257480, 0.5497884204, 0.6710426295, 0.8191385439, 1.]

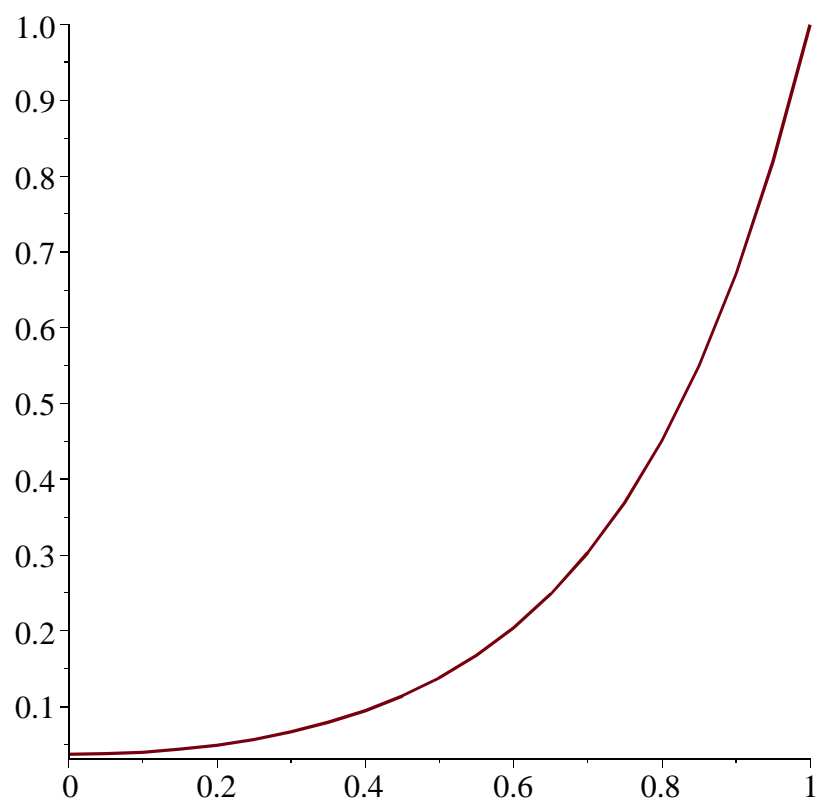
"iterace = ", 2, " s = ", $9.712016986 \cdot 10^{-10}$

"y = ", [0.03678801686, 0.03753879272, 0.03979112029, 0.04363509266, 0.04922446874, 0.05678282357, 0.06661249135, 0.07910665878, 0.09476509256, 0.1142141300, 0.1382317327, 0.1677786047, 0.2040366209, 0.2484561019, 0.3028138270, 0.3692841052, 0.4505257476, 0.5497884199, 0.6710426292, 0.8191385436, 1.]

(3.11)

```
> # Graf funkce y(x)
```

```
> plot(yres);
```

```
> # Tabulka hodnot funkce y(x)  
> linalg[matrix](yres);
```

(3.12)

--	--

0.	0.03678801686
0.05000000000	0.03753879272
0.10000000000	0.03979112029
0.15000000000	0.04363509266
0.20000000000	0.04922446874
0.25000000000	0.05678282357
0.30000000000	0.06661249135
0.35000000000	0.07910665878
0.40000000000	0.09476509256
0.45000000000	0.1142141300
0.50000000000	0.1382317327
0.55000000000	0.1677786047
0.60000000000	0.2040366209
0.65000000000	0.2484561019
0.70000000000	0.3028138270
0.75000000000	0.3692841052
0.80000000000	0.4505257476
0.85000000000	0.5497884199
0.90000000000	0.6710426292
0.95000000000	0.8191385436
1.0000000000	1.

(3.12)