Example 3.

Sensitivity of hydraulic head at a point to Dirichlet BC head under steady state flow conditions

0. Forward model

Governing equation:

$$K\,b\,\frac{d^2h}{dx^2}+R=0 \tag{1}$$

$$\tag{2}$$

Boundary conditions:

$$-K\,b\,\frac{dh(x)}{dx}=0\,, \qquad x=0=\Gamma_2 \tag{3}$$

$$h(x)=h_{\Gamma_1}\,, \qquad x=L=\Gamma_1 \tag{4}$$

$$\tag{5}$$

Closed-form solution:

$$h(x)=h_L+\frac{R(L^2-x^2)}{2\,K\,b} \tag{6}$$

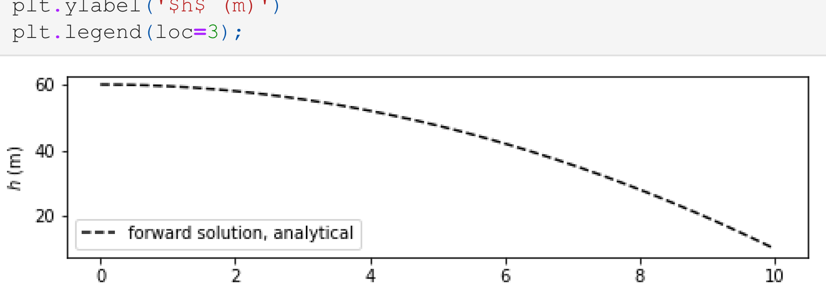
$$\tag{7}$$

Spatial derivatives from differentiation:

$$\frac{dh}{dx}=-\frac{R\,x}{K\,b}, \qquad \frac{d^2h}{dx^2}=-\frac{R}{K\,b} \tag{8}$$

In [45]:
```
from IPython.display import HTML, display
def set_background(color):
    script = (
        "var cell = this.closest('.code_cell');"
        "var editor = cell.querySelector('.input_area');"
        "editor.style.background='{}';"
        "this.parentNode.removeChild(this)").format(color)
    display(HTML('<img src onerror="{}">'.format(script)))
```

In [46]:
```
from warnings import filterwarnings
filterwarnings("ignore", category=DeprecationWarning)

import numpy as np

def h(x, K, R, b, L, BC1h):
    return BC1h+R/K/2./b*(L**2.-x**2.)

K, R, b, L, BC1h, ocol = 10., 1e-1/1000., 10., 10000., 10., 5000
X = np.arange(L)
H0 = np.array([h(x, K, R, b, L, BC1h) for x in X])

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., H0, 'k--', mfc='none', label='forward solution, analytical')
plt.xlabel('$x$ (km)')
plt.ylabel('$h$ (m)')
plt.legend(loc=3);
```



1. Direct sensitivity

$$\tag{9}$$

$$\frac{\partial h(x')}{\partial h_{\Gamma_1}}=1 \tag{10}$$

$$\tag{11}$$

In [47]:
```
set_background('rgba(0, 200, 0, 0.2)')
benchmark = 1.
```

2. Perturbation sensitivity

$$\tag{12}$$

$$\frac{\partial h(x')}{\partial h_{\Gamma_1}}\approx\frac{h(x,h_{\Gamma_1}+\Delta h_{\Gamma_1})-h(x,h_{\Gamma_1})}{\Delta h_{\Gamma_1}} \tag{13}$$

$$\tag{14}$$

2a. Analytical

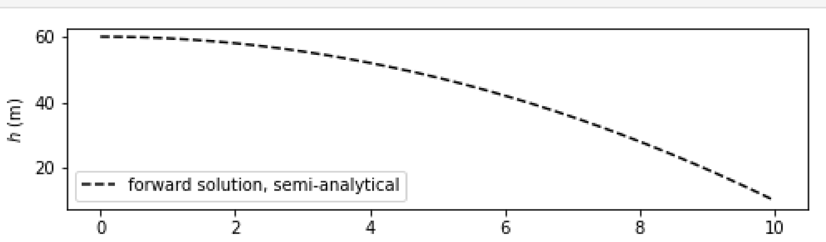
In [48]:
```
dpar = 1e-0
H0 = np.array([h(x, K, R, b, L, BC1h) for x in X])
H1 = np.array([h(x, K, R, b, L, BC1h+BC1h*dpar) for x in X])
dhdBC1h = (H1-H0)/(BC1h*dpar)

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC1h, 'k--', mfc='none', label='perturbation sensitivity, analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial h_{\Gamma_1}$')
plt.legend()
plt.ylim(0.95, 1.05);
```

In [49]:
```
set_background('rgba(0, 200, 0, 0.2)')
print('%.6f (%.6f)'% (dhdBC1h[ocol], benchmark))
```

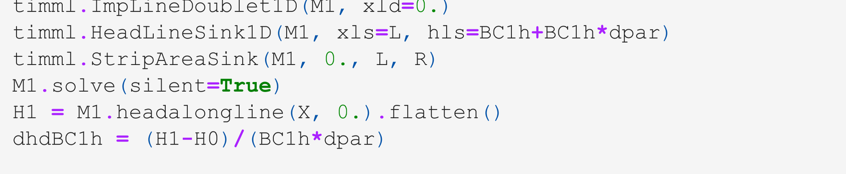
```
1.000000 (1.000000)
```

2b. Semi-analytical

In [50]:
```
from os import getcwd, chdir
cwd = getcwd()
chdir(r'../../timml')
import timml
chdir(cwd)

M0 = timml.Model3D(kaq=K, z=[0., -b])
timml.ImpLineDoublet1D(M0, xld=0.)
timml.HeadLineSink1D(M0, xls=L, hls=BC1h)
timml.StripAreaSink(M0, 0., L, R)
M0.solve(silent=True)
H0 = M0.headalongline(X, 0.).flatten()

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., H0, 'k--', mfc='none', label='forward solution, semi-analytical')
plt.xlabel('$x$ (km)')
plt.ylabel('$h$ (m)')
plt.legend(loc=3);
```



In [51]:
```
M1 = timml.Model3D(kaq=K, z=[0., -b])
timml.ImpLineDoublet1D(M1, xld=0.)
timml.HeadLineSink1D(M1, xls=L, hls=BC1h+BC1h*dpar)
timml.StripAreaSink(M1, 0., L, R)
M1.solve(silent=True)
H1 = M1.headalongline(X, 0.).flatten()
dhdBC1h = (H1-H0)/(BC1h*dpar)

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC1h, 'k--', mfc='none', label='perturbation sensitivity, semi-analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial h_{\Gamma_1}$')
plt.legend()
plt.ylim(0.95, 1.05);
```

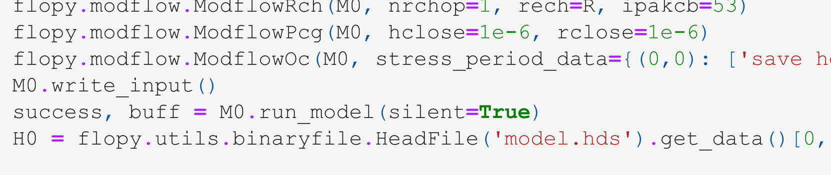


In [52]:
```
set_background('rgba(0, 200, 0, 0.2)')
print('%.6f (%.6f)'% (dhdBC1h[ocol], benchmark))
```

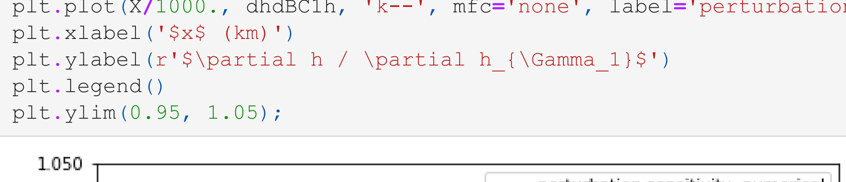
```
1.000000 (1.000000)
```

2c. Numerical

In [53]:
```
import flopy

nrow, ncol = 1, int(L)
M0 = flopy.modflow.Modflow(modelname='model', exe_name='../mf2005.exe')
flopy.modflow.ModflowDis(M0, nlay=1, nrow=nrow, ncol=ncol, nper=1, delr=1., delc=1., top=0., botm=-b, steady=Tr
                         perlen=1., nstp=1)
flopy.modflow.ModflowBas(M0, ibound=np.hstack([np.ones([nrow, ncol-1], dtype=int), -1*np.ones([1,1])]),
                         strt=BC1h*np.ones([nrow, ncol], dtype=float))
flopy.modflow.ModflowLpf(M0, hk=K, vka=-999., ss=-999., sy=-999., ipakcb=53)
flopy.modflow.ModflowRch(M0, nrchop=1, rech=R, ipakcb=53)
flopy.modflow.ModflowPcg(M0, hclose=1e-6, rclose=1e-6)
flopy.modflow.ModflowOc(M0, stress_period_data={(0,0): ['save head', 'save budget']})
M0.write_input()
success, buff = M0.run_model(silent=True)
H0 = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., H0, 'k--', mfc='none', label='forward solution, numerical')
plt.xlabel('$x$ (km)')
plt.ylabel('$h$ (m)')
plt.legend(loc=3);
```



In [54]:
```
M1 = M0
flopy.modflow.ModflowBas(M1, ibound=np.hstack([np.ones([nrow, ncol-1], dtype=int), -1*np.ones([1,1])]),
                         strt=(BC1h+BC1h*dpar)*np.ones([nrow, ncol], dtype=float))
M1.write_input()
success, buff = M1.run_model(silent=True)
H1 = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]
dhdBC1h = (H1-H0)/(BC1h*dpar)

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC1h, 'k--', mfc='none', label='perturbation sensitivity, numerical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial h_{\Gamma_1}$')
plt.legend()
plt.ylim(0.95, 1.05);
```



In [55]:
```
set_background('rgba(0, 200, 0, 0.2)')
print('%.6f (%.6f)'% (dhdBC1h[ocol], benchmark))
```

```
1.000000 (1.000000)
```

3. Adjoint sensitivity

$$\frac{\partial h(x')}{\partial h_{\Gamma_1}}=-\int_{\Gamma_1}K\frac{d\psi_1^*(x)}{dx}\,dx\;=\;K\frac{d\psi_1^*}{dx}(\Gamma_1)\;=\;q\,(\Gamma_1) \tag{15}$$

Governing equation:

$$K\,b\,\frac{d\psi_1^*}{dx}+\frac{1}{2\,K\,b}\delta(x-x')=0 \tag{16}$$

$$\tag{17}$$

Boundary conditions:

$$-K\,b\,\frac{d\psi_1^*(x)}{dx}=0\,, \qquad x=0=\Gamma_2 \tag{18}$$

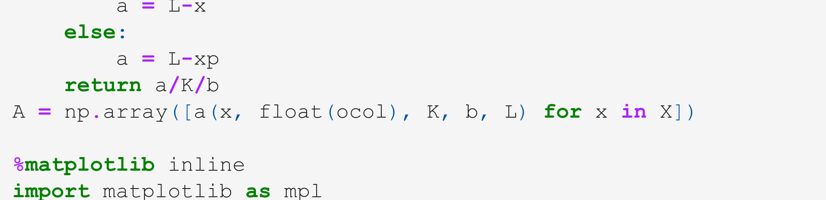
$$\psi_1^*(x)=0\,, \qquad x=L=\Gamma_1 \tag{19}$$

$$\tag{20}$$

Closed-form solution:

$$\psi_1^*(x)=\frac{1}{2\,K\,b}\left[H\left(x'-x\right)\left(L-x'\right)+H\left(x-x'\right)\left(L-x\right)\right] \tag{21}$$

In [56]:
```
def a(x, xp, K, b, L):
    if x>xp:
        a = L-x
    else:
        a = L-xp
    return a/K/b
A = np.array([a(x, float(ocol), K, b, L) for x in X])

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., A, 'k--', mfc='none', label='adjoint solution, analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\psi^*_1$ (T/$L^2$)')
plt.legend(loc=3);
```



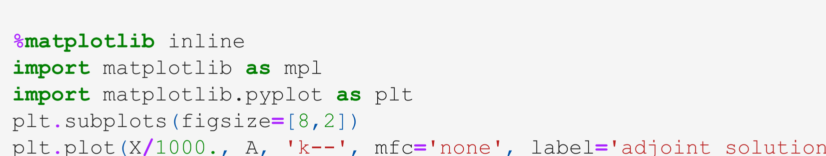
3a. Analytical

$$\frac{d\psi_1^*}{dx}=-\frac{1}{2\,K\,b} \tag{22}$$

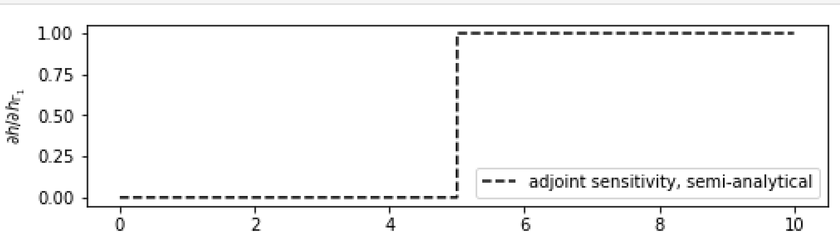
$$\therefore K\frac{d\psi_1^*(x)}{dx}=-\frac{1}{2\,b} \tag{23}$$

3b. Semi-analytical

In [58]:
```
M0 = timml.Model3D(kaq=K, z=[0., -b])
timml.ImpLineDoublet1D(M0, xld=0.)
timml.HeadLineSink1D(M0, xls=L, hls=0.)
timml.LineSink1D(M0, xls=float(ocol), sigls=-1.)
M0.solve(silent=True)
A = M0.headalongline(X, 0.).flatten()

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., A, 'k--', mfc='none', label='adjoint solution, semi-analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\psi^*_1$ (T/$L^2$)')
plt.legend(loc=3);
```



In [59]:
```
dhdBC1h = np.array([M0.disvec(x,0) for x in X])[:,0].flatten()

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
f,s = plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC1h, 'k--', mfc='none', label='adjoint sensitivity, semi-analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial h_{\Gamma_1}$')
plt.legend(loc=4);
```

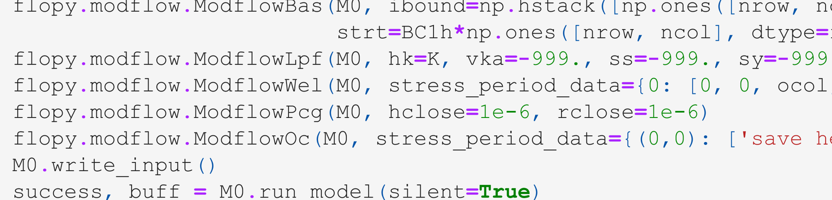


In [60]:
```
set_background('rgba(0, 200, 0, 0.2)')
print('%.6f (%.6f)'% (dhdBC1h[-1], benchmark))
```

```
1.000000 (1.000000)
```

3c. Numerical

In [61]:
```
M0 = flopy.modflow.Modflow(modelname='model', exe_name='../mf2005.exe')
flopy.modflow.ModflowDis(M0, nlay=1, nrow=1, ncol=ncol, nper=1, delr=1., delc=1., top=0., botm=-b, steady=True,
                         perlen=1., nstp=1)
flopy.modflow.ModflowBas(M0, ibound=np.hstack([np.ones([nrow, ncol-1], dtype=int), -1*np.ones([1,1])]),
                         strt=BC1h*np.ones([nrow, ncol], dtype=float))
flopy.modflow.ModflowLpf(M0, hk=K, vka=-999., ss=-999., sy=-999., ipakcb=53)
flopy.modflow.ModflowWel(M0, stress_period_data={0: [0, 0, ocol, 1.]})
flopy.modflow.ModflowPcg(M0, hclose=1e-6, rclose=1e-6)
flopy.modflow.ModflowOc(M0, stress_period_data={(0,0): ['save head', 'save budget']})
M0.write_input()
success, buff = M0.run_model(silent=True)
A = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., A, 'k--', mfc='none', label='adjoint solution, numerical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\psi^*_1$ (T/$L^2$)')
plt.legend(loc=3);
```



In [62]:
```
dhdBC1h = np.array(flopy.utils.binaryfile.CellBudgetFile('model.cbc').get_data(text='CONSTANT HEAD')).flatten()

'''%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC1h, 'k--', mfc='none', label='adjoint sensitivity, numerical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'K $d\psi^*_1 / dx$')
plt.legend()''';
```

In [63]:
```
set_background('rgba(0, 200, 0, 0.2)')
print('%.6f (%.6f)'% (dhdBC1h[0][1], benchmark))
```

```
-1.000000 (1.000000)
```

In [ ]: