Example 5.

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

0. Forward model

Governing equation:

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

$$\tag{2}$$

Boundary conditions:

$$q(x) = q_{\Gamma_2}\ , \qquad x = 0 = \Gamma_2 \tag{3}$$

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

$$\tag{5}$$

Closed-form solution:

$$\text{Not available} \tag{6}$$

$$\tag{7}$$

Spatial derivatives from differentiation:

$$\text{Not available} \tag{8}$$

In [92]:

```
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 [93]:

```
from warnings import filterwarnings
filterwarnings("ignore", category=DeprecationWarning)

import numpy as np

K, b, L, BC1h, BC2q, ocol = 10., 10., 10000., 0., 0.5, 5000
X = np.arange(L)
```

1. Direct sensitivity

$$\tag{9}$$

$$\text{Not available} \tag{10}$$

$$\tag{11}$$

In [ ]:

2. Perturbation sensitivity

$$\tag{12}$$

$$\frac{\partial h(x')}{\partial q_{\Gamma_2}} \approx \frac{h(x, q_{\Gamma_2} + \Delta q_{\Gamma_2}) - h(x, q_{\Gamma_2})}{\Delta q_{\Gamma_2}} \tag{13}$$

$$\tag{14}$$

2a. Analytical

$$\tag{15}$$

$$\text{Not available} \tag{16}$$

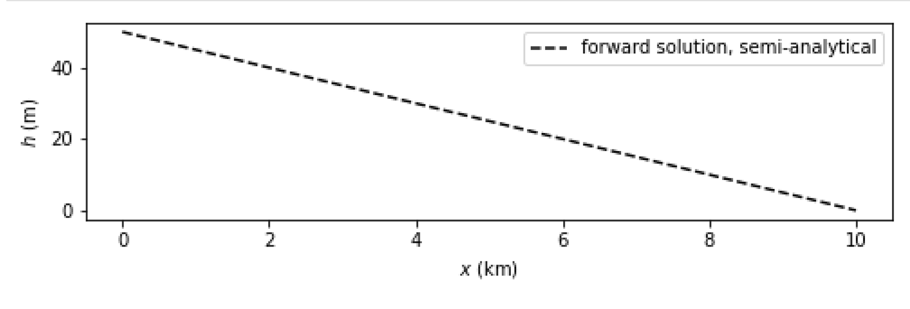
$$\tag{17}$$

In [ ]:

2b. Semi-analytical

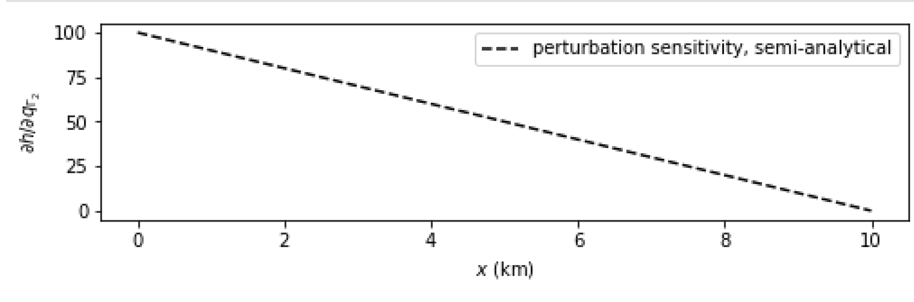
In [94]:

```
from os import getcwd, chdir
cwd = getcwd()
chdir(r'../../timml')
import timml
chdir(cwd)

dpar = 1e-4
M0 = timml.Model3D(kaq=K, z=[0., -b])
timml.LineSink1D(M0, xls=0, sigls=-BC2q/5000.)
timml.HeadLineSink1D(M0, xls=L, hls=0.)
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();
```



In [95]:

```
M1 = timml.Model3D(kaq=K, z=[0., -b])
timml.LineSink1D(M1, xls=0, sigls=-BC2q/5000.-BC2q/5000.*dpar)
timml.HeadLineSink1D(M1, xls=L, hls=0.)
M1.solve(silent=True)
H1 = M1.headalongline(X, 0.).flatten()
dhdBC2q = (H1-H0)/(BC2q*dpar)

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC2q, 'k--', mfc='none', label='perturbation sensitivity, semi-analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial q_{\Gamma_2}$')
plt.legend();
```



In [96]:

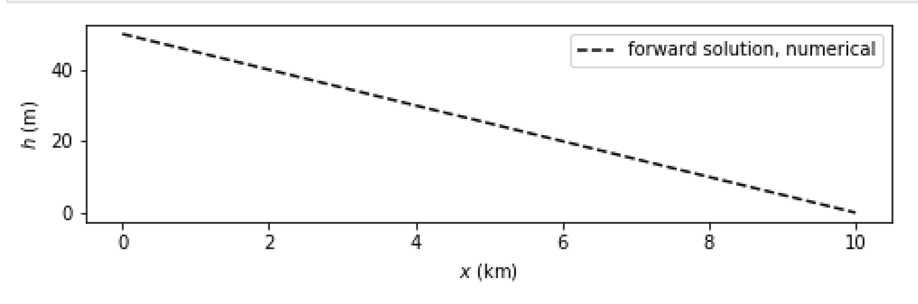
```
print('%.6f'% dhdBC2q[ocol])
```

```
50.010000
```

2c. Numerical

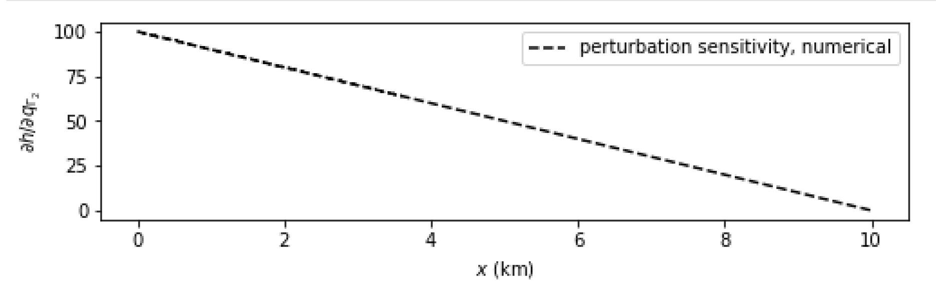
In [97]:

```
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.ModflowWel(M0, stress_period_data={0: [0, 0, 0, BC2q]})
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();
```



In [98]:

```
M1 = M0
flopy.modflow.ModflowWel(M1, stress_period_data={0: [0, 0, 0, BC2q+BC2q*dpar]})
M1.write_input()
success, buff = M1.run_model(silent=True)
H1 = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]
dhdBC2q = (H1-H0)/(BC2q*dpar)

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X/1000., dhdBC2q, 'k--', mfc='none', label='perturbation sensitivity, numerical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial q_{\Gamma_2}}$')
plt.legend();
```



In [99]:

```
print('%.6f'% dhdBC2q[ocol])
```

```
49.972534
```

3. Adjoint sensitivity

$$\frac{\partial h(x')}{\partial q_{\Gamma_2}} = \oint_{\Gamma_2} \psi_1^*(x)\ dx\ =\ \psi_1^*(\Gamma_2) \tag{18}$$

Governing equation:

$$K\,b\,\frac{d\psi_1^*}{dx} + \frac{1}{2\,K\,b}\delta(x - x') = 0 \tag{19}$$

$$\tag{20}$$

Boundary conditions:

$$\psi_1^*(x) = 0\ , \qquad x = 0 = \Gamma_{1_0} \tag{21}$$

$$\psi_1^*(x) = 0\ , \qquad x = L = \Gamma_{1_L} \tag{22}$$

$$\tag{23}$$

Closed-form solution:

$$\text{Not available} \tag{24}$$

In [ ]:

3a. Analytical

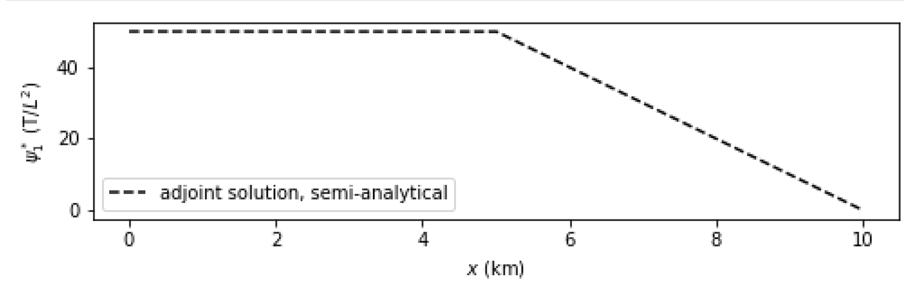
$$\text{Not available} \tag{25}$$

In [ ]:

3b. Semi-analytical

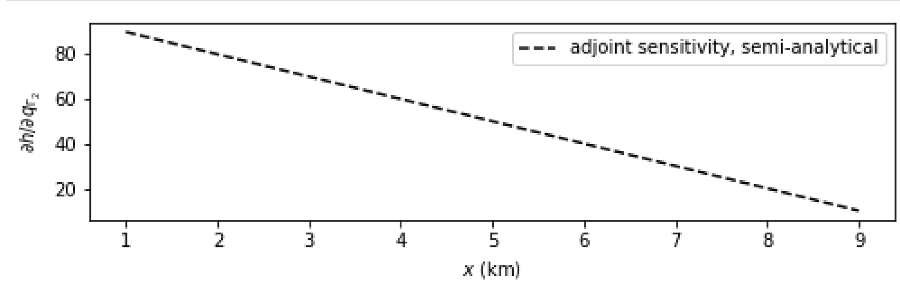
In [100…

```
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 [102…

```
dhdBC2q = np.empty(0)
for xp in X[::1000]:
    M0 = timml.Model3D(kaq=K, z=[0., -b])
    timml.ImpLineDoublet1D(M0, xld=0.)
    timml.HeadLineSink1D(M0, xls=L, hls=0.)
    timml.LineSink1D(M0, xls=xp, sigls=-1.)
    M0.solve(silent=True)
    A = M0.headalongline(X, 0.).flatten()
    dhdBC2q = np.append(dhdBC2q, A[0])

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.subplots(figsize=[8,2])
plt.plot(X[::1000][1:]/1000., dhdBC2q[1:], 'k--', mfc='none', label='adjoint sensitivity, semi-analytical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial q_{\Gamma_2}$')
plt.legend();
```



In [103…

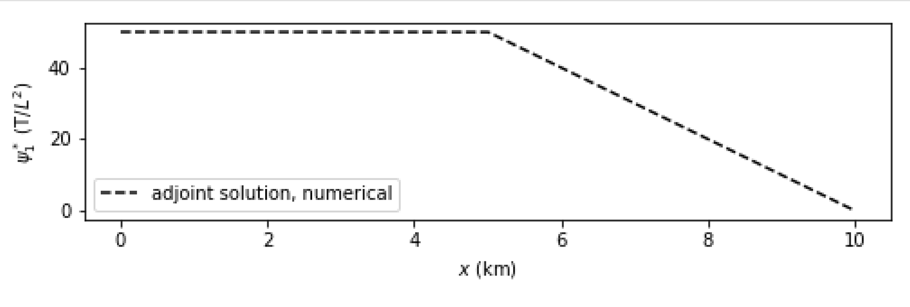
```
print('%.6f'% dhdBC2q[int(np.where(X[::1000]==float(ocol))[0])])
```

```
50.000000
```

3c. Numerical

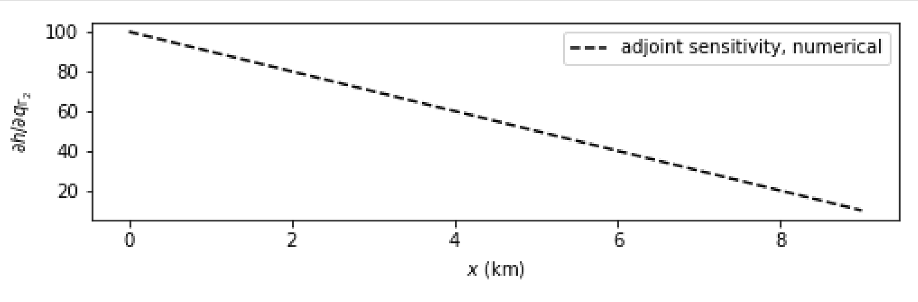
In [107…

```
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 [110…

```
dhdBC2q = np.empty(0)
for oc,xp in enumerate(X[::1000]):
    M1 = M0
    flopy.modflow.ModflowWel(M0, stress_period_data={0: [0, 0, oc*1000, 1.]})
    M0.write_input()
    success, buff = M0.run_model(silent=True)
    A = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]
    dhdBC2q = np.append(dhdBC2q, A[0])

%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
f,s = plt.subplots(figsize=[8,2])
plt.plot(X[::1000]/1000., dhdBC2q, 'k--', mfc='none', label='adjoint sensitivity, numerical')
plt.xlabel('$x$ (km)')
plt.ylabel(r'$\partial h / \partial q_{\Gamma_2}$')
plt.legend();
```



In [112…

```
print('%.6f'% dhdBC2q[int(np.where(X[::1000]==float(ocol))[0])])
```

```
49.990002
```

In [ ]: