A Simulation Software for Contaminant Spreading

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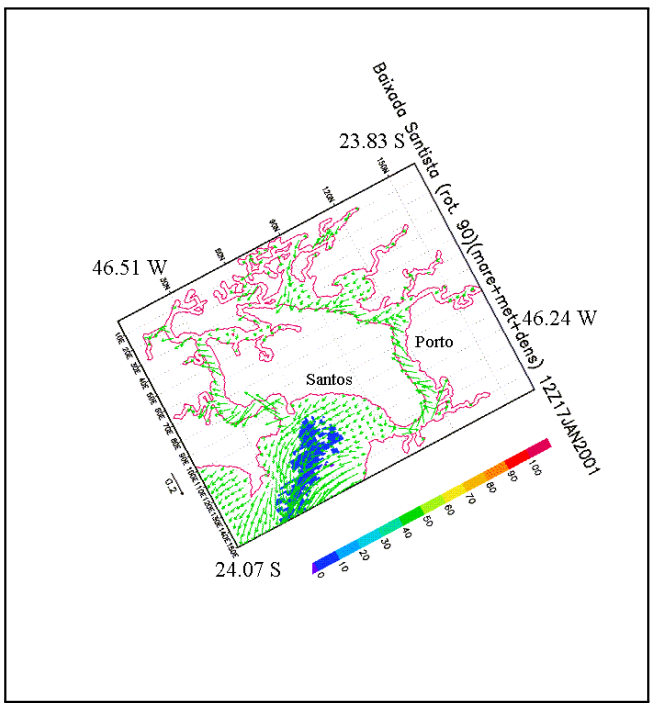
Motivation

- Transport of chemical species in natural water is ubiquitous.
- Tailor-made solutions, e.g. Excel spreadsheets,
- Standardized softwares (EPA): QUAL2K, WASP, CORMIX
- Common features: input values through dialogs



(Harari et al., 2004)

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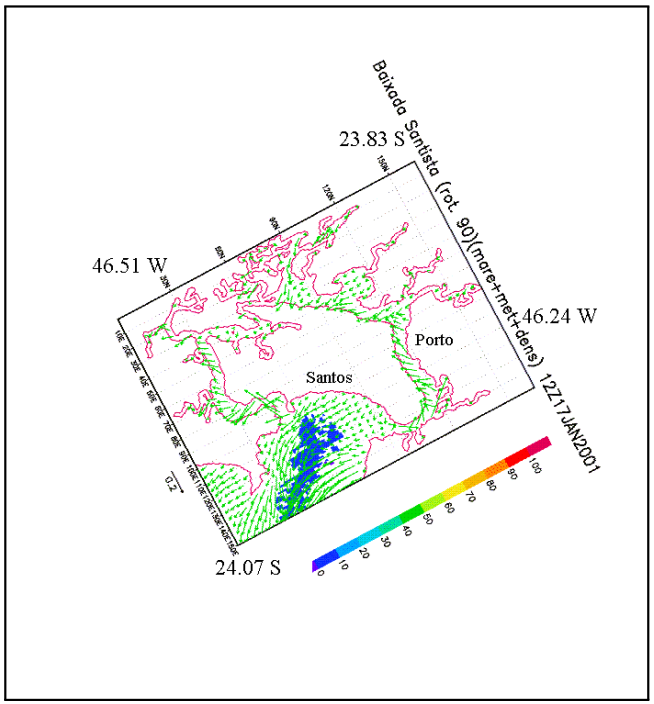


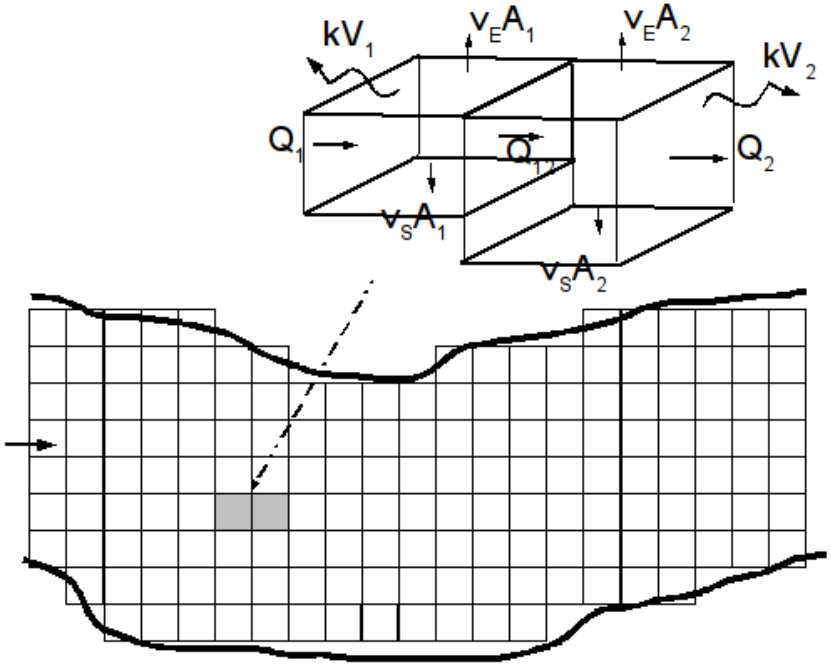
(Harari et al., 2004)

Why make another software?

- Revise the conceptual model
- Implement numerical calculation
- Visualize result the way we like
- Programming is enjoyable :)

The geometrical domain

$$V\Delta c/\Delta t = \Sigma W + \Sigma Q_{in} c_i - \Sigma Q_{out} c + \Sigma E(c_i - c) - k' V c$$

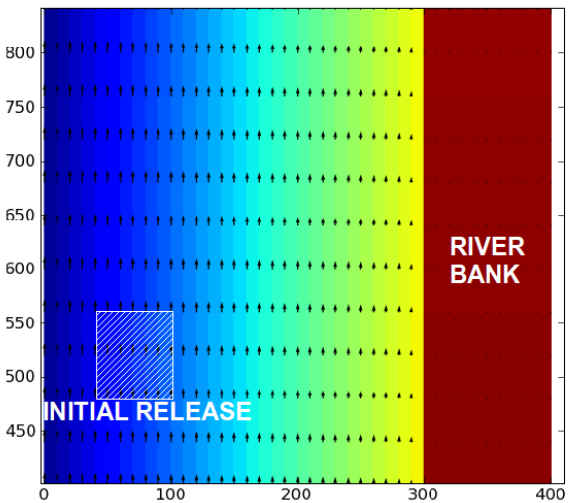


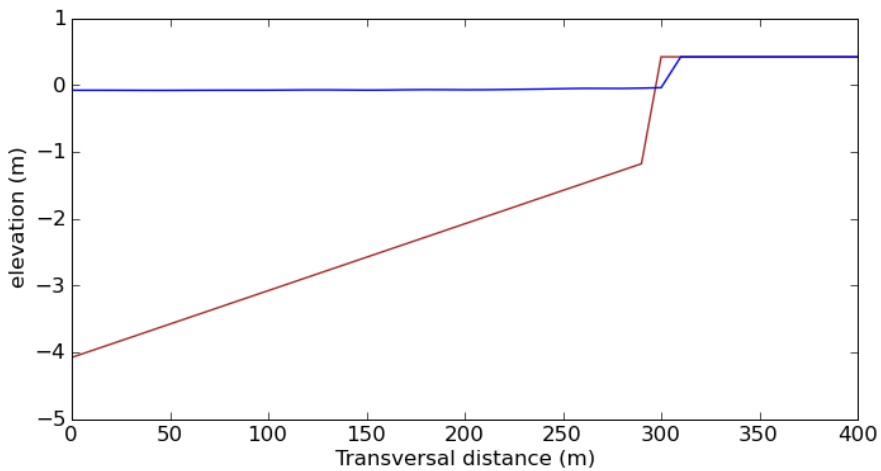
- 2-D horizontal domain
- Control volume dimensions: $\Delta x \times \Delta y \times h$
- Staggered grid
- Within-cell variables: c, h, z_b
- Inter-cell variables: u, v
- Universal parameters: k, E, Ch

The solver

Solver ▷ Interface

- Flow solver – Concentration add-on
- Vectorized coding, based on XBeach `http://xbeach.org/`
- Test case: Simple straight channel, steady flow (advection)





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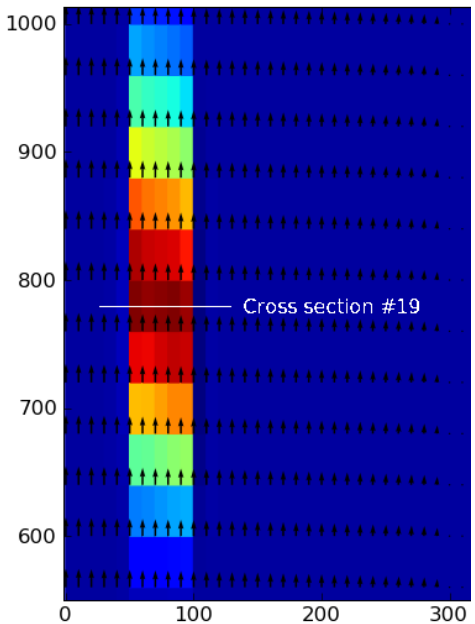

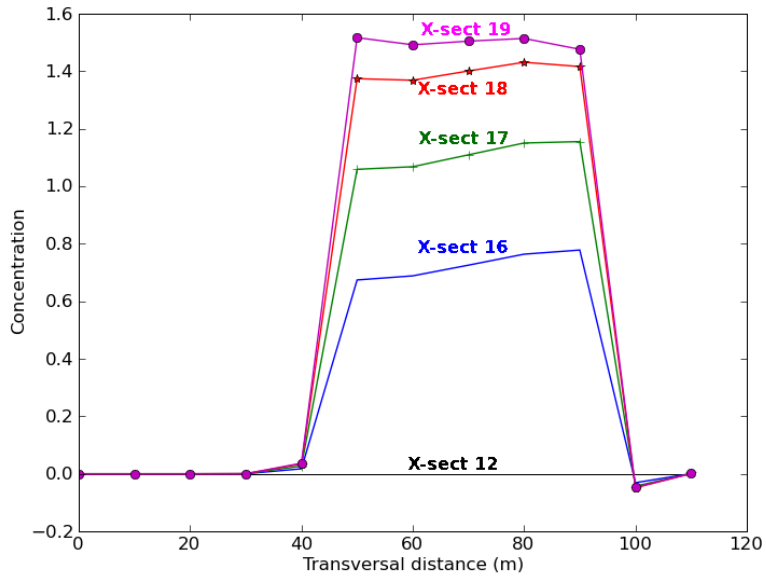

The solver

Solver ▷ Interface

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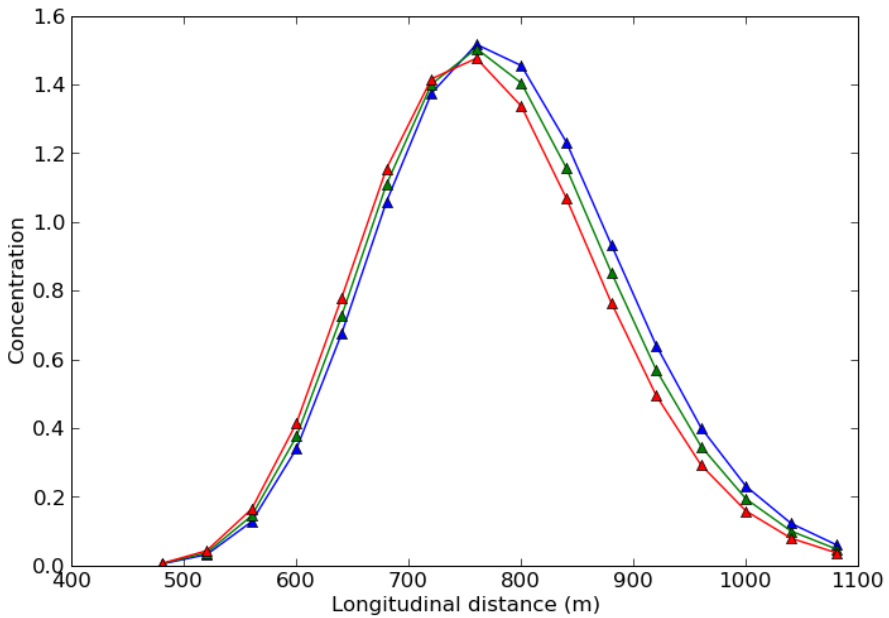
Conc. profiles along river

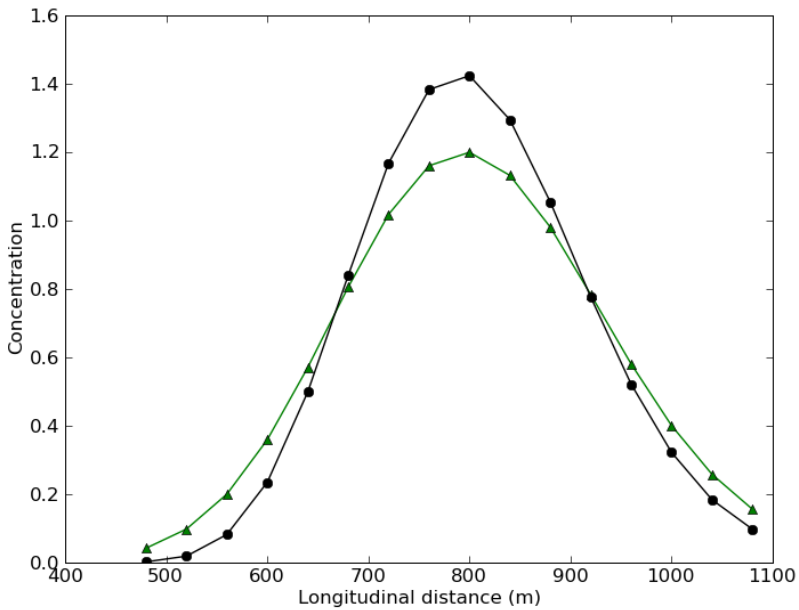


The solver

Solver ▷ Interface

- Flow solver – Concentration add-on
- Vectorized coding, based on XBeach `http://xbeach.org/`
- Test case: Simple straight channel, steady flow (+ diffusion)

- $E_{long} = 10\ \mathrm{m}^2/\mathrm{s}$
- $E_{tran} = 0.1\ \mathrm{m}^2/\mathrm{s}$
- $Pe \sim O(1)$



Interface

Solver ▷ Interface

- Get/prescribe variable values from the solver during simulation

```
h[i,j], zs[i,j], u[i,j], v[i,j]
-h[100,:], zs[:,100]
u * (u > 0.01)
```

Interface

Solver ▷ Interface

- Get/prescribe variable values from the solver during simulation

```
h[i,j], zs[i,j], u[i,j], v[i,j]
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u * (u > 0.01)
```

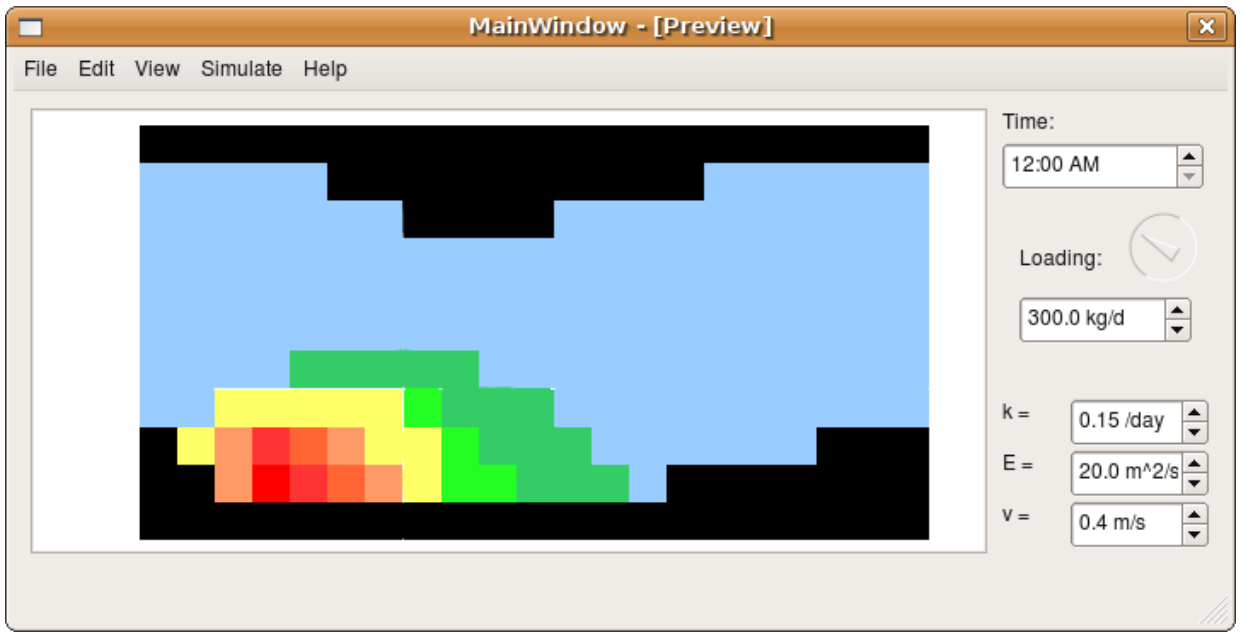
- Loading can be modified in case of steady flow!

```
W[84:87,61:65] = 5
for i = 1, 5 do solve()
W[84:87,61:65] = 0
for i = 1, 5 do solve()
```

User Interface and Input/Output

Solver ▷ Interface

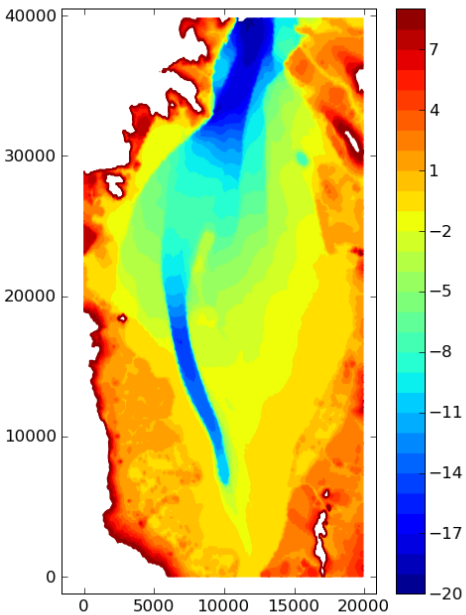
- Graphical UI: Display window, Spinboxes, Sliders, Menus
- To do: menus, scenarios
- One data file for parameters and variables
- "Hot-starts" !

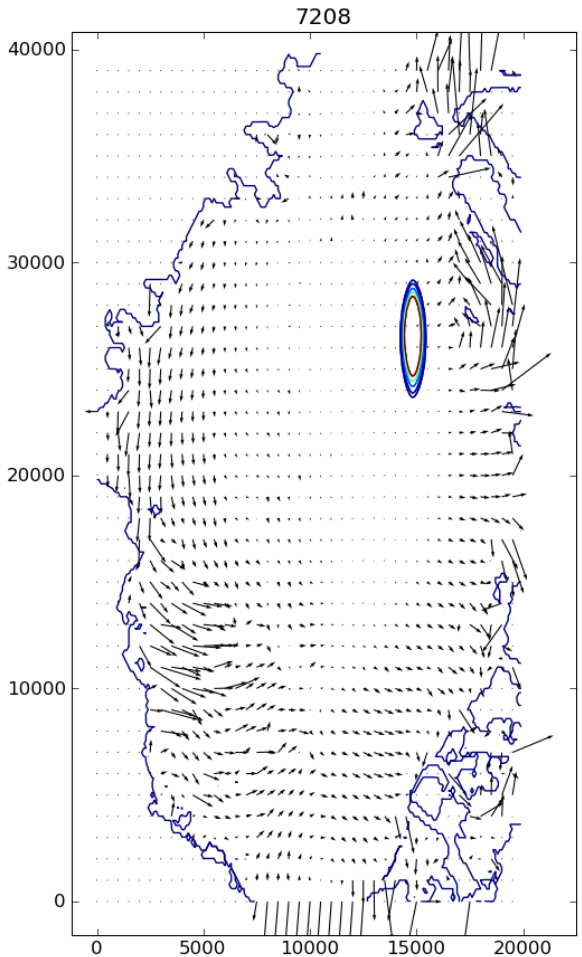


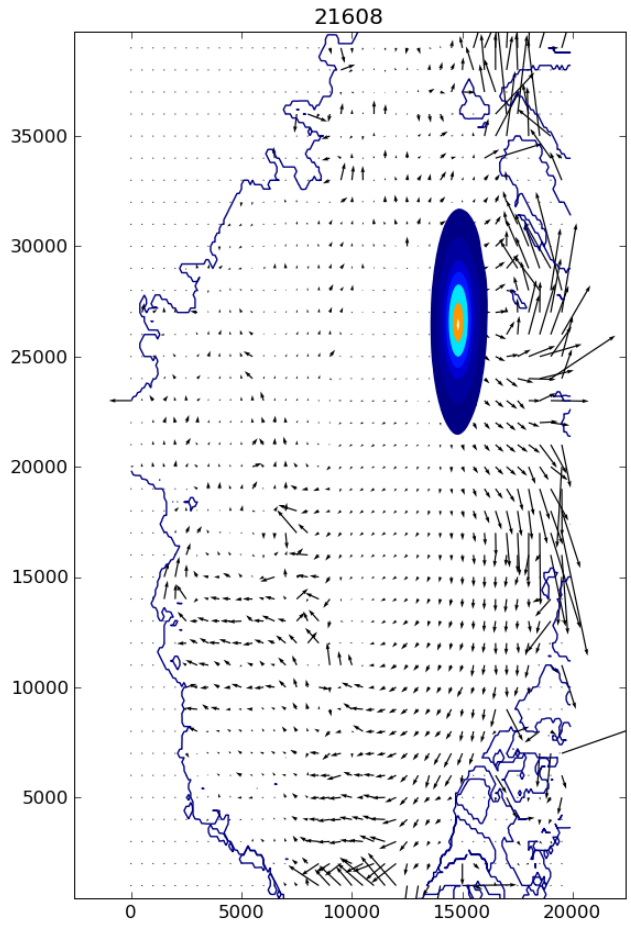
Simulation for San Francisco Bay

- Dimension: ≈ 40 km $\times$ 10 km
- $\mathtt{nx} = 200, \mathtt{ny} = 200$
- $\Delta x = 200$ m, $\Delta y = 100$ m.
- boundaries, calibration, sites.
- Bathymetry: DEM 3".
- Simulation for: 22-Jun-2009
- Boundaries: water levels (Tide / NOAA)
- Loading: at site A (132, 148) $W = 38.08$ g/s

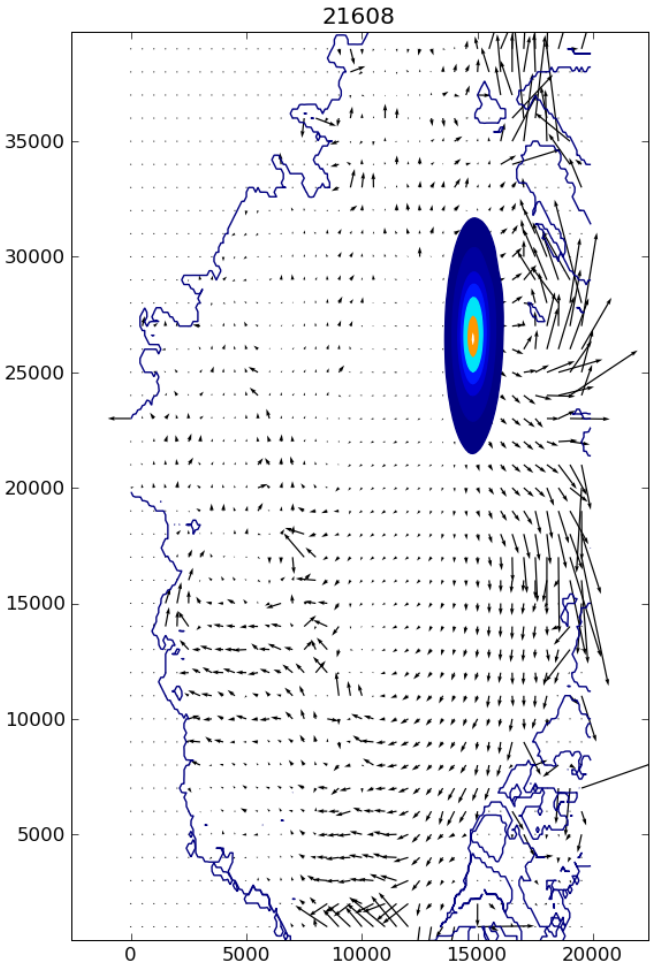
Result

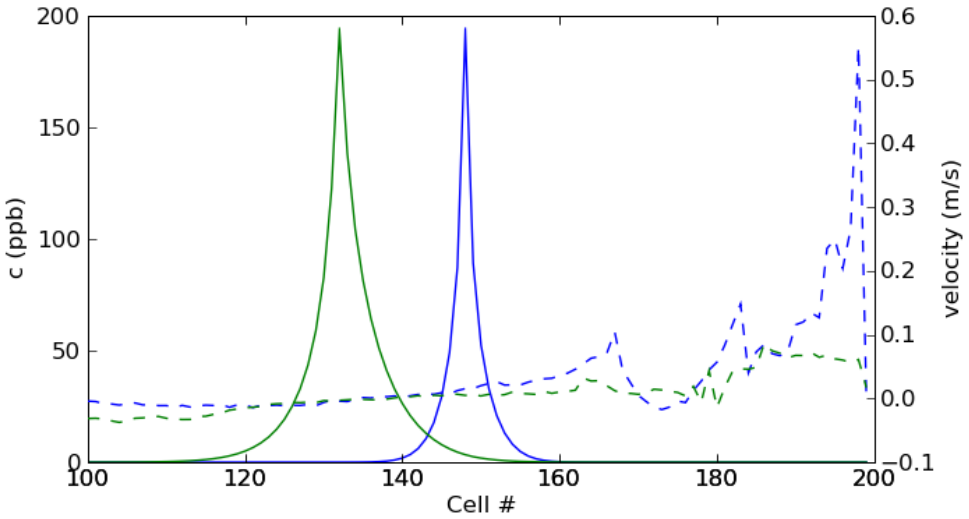

40000
30000
20000
10000
0
0
5000
10000
15000
20000
7
4
1
−2
−5
−8
−11
−14
−17
−20

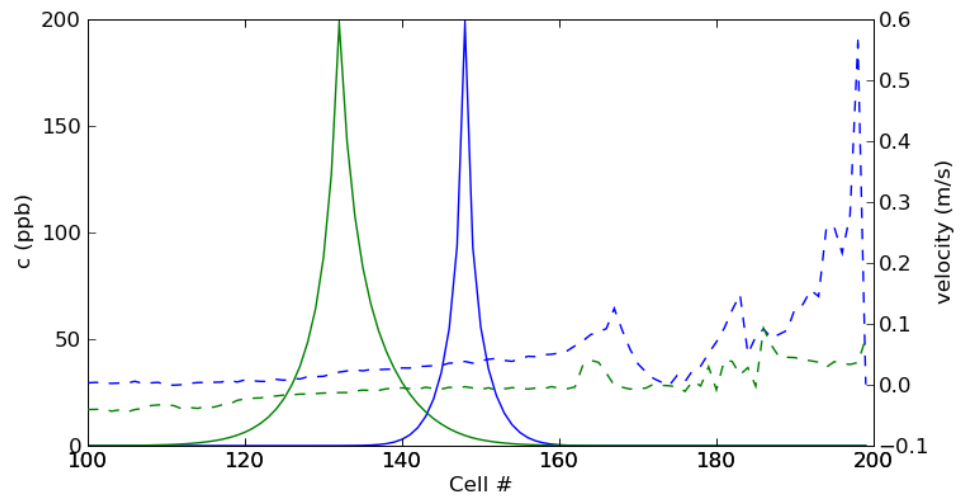

7208
40000
30000
20000
10000
0
0
5000
10000
15000
20000


21608
35000
30000
25000
20000
15000
10000
5000
0
5000
10000
15000
20000

Result (2)


21608
35000
30000
25000
20000
15000
10000
5000
0
5000
10000
15000
20000


200
150
100
50
0
c (ppb)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
velocity (m/s)
100
120
140
160
180
200
Cell #


200
150
100
50
0
c (ppb)
0.6
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0.4
0.3
0.2
0.1
0.0
−0.1
velocity (m/s)
100
120
140
160
180
200
Cell #

What have we discussed?

- Simulation tool for contaminant transport
- Interactive input dialog and display
- Scope: shallow water, 2D
- Advection / diffusion similar to textbook formulae
- Simulation of pollutant spreading in S.F. bay
- Visit `http://code.google.com`

Chapra, S. C., 1997. *Surface Water-Quality Modeling*, McGraw-Hill, 844 pp.

Fischer, H. B., 1979. *Mixing in Inland and Coastal Waters*, Academic Press, 483 pp.

Harari, J. & de Camargo, R. & de Sampaio Franca, C. A. & Monteiro, M. Q. Modeling the circulation and dispersion in Santos coastal region (SP, Brazil): applications to impacted and preserved areas. `http://www.mares.io.usp.br/aagn/7/jh/aagn2004disp_laje_jh.htm`