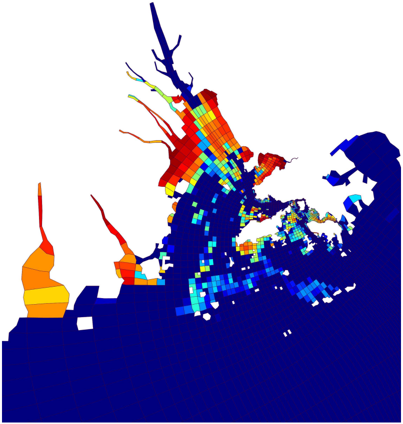
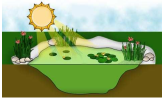
A Robust Higher-Order Variable-θ Scheme for the Advection Diffusion Equation on Unstructured Grids



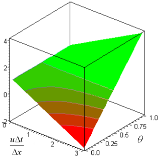
Paulien van Slingerland
WL Delft Hydraulics & Delft University of Technology
March 27, 2007

Domestic and industrial waste waters constitute a major source of **water pollution** near Hong Kong

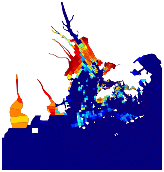
Outline of the presentation:



Delft3D-WAQ simulates water quality



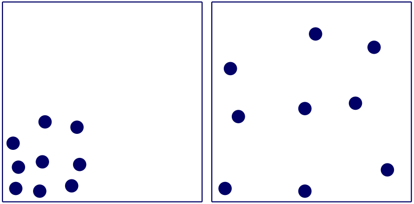
The **problem** involves the relation between numerical diffusion and computational speed



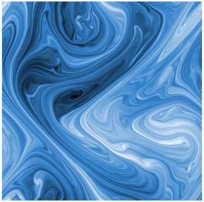
The **solution** is to manage 'nice properties' with a parameter, rather than with the time step

Water quality is determined by **transport** and water quality processes

Molecular diffusion



Turbulent mixing

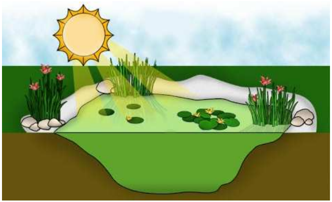


Advection

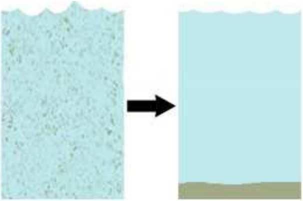
Other Transport

Water quality is determined by transport and **water quality processes**

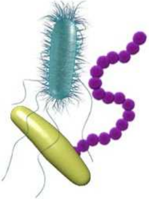
Fotosynthesis



Sedimentation



Mortality of Bacteria



Algal Growth

Delft3D-WAQ simulates water quality by solving the **advection-diffusion equation** by means of the FVM

$$\underbrace{\frac{\partial c}{\partial t}}_{\text{change}} = \underbrace{-\nabla \cdot (\underline{\mathbf{u}} c - d \nabla c)}_{\text{transport}} + \underbrace{p}_{\text{processes}}$$

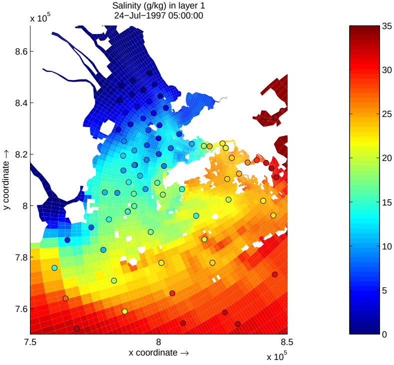
c	concentration
$\underline{\mathbf{u}}$	velocity
d	diffusion coefficient
p	water quality processes

The **problem** is that WAQ's current finite volume schemes are either too **inaccurate** or too **expensive**

implicit first order upwind

$\Delta t = 20\,\mathrm{min.}$

simulation time $= 20\,\mathrm{min.}$

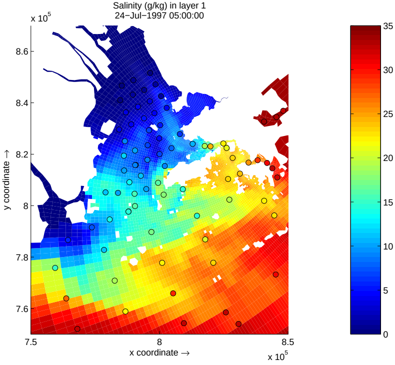


too diffusive

explicit FCT (Boris & Book)

$\Delta t = 1\,\mathrm{min.}$

simulation time $= 176\,\mathrm{min.}$

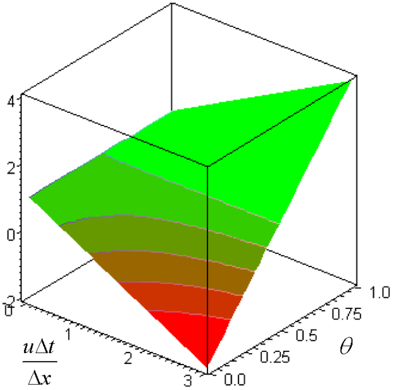


too much CPU-time

The **numerical diffusion coefficient** of the upwind-θ scheme for the 1d advection equation reveals the **cause**

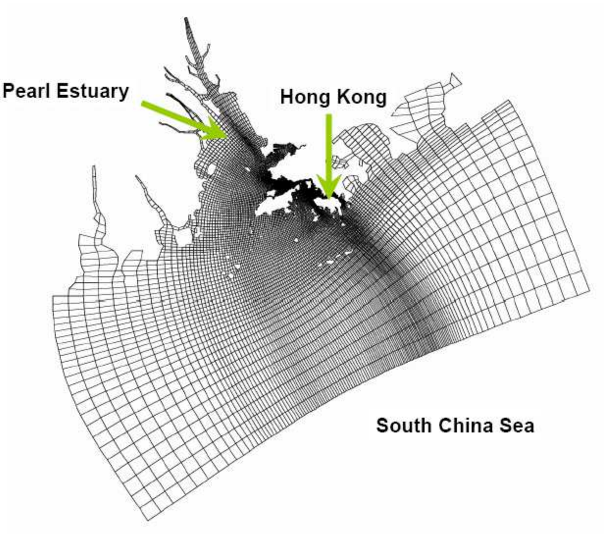
$$\text{num. diff.} \;=\; \frac{u\Delta x}{2}\underbrace{\left(1-(1-2\theta)\frac{u\Delta t}{\Delta x}\right)}$$

stable
diffusive
small Δt
large θ



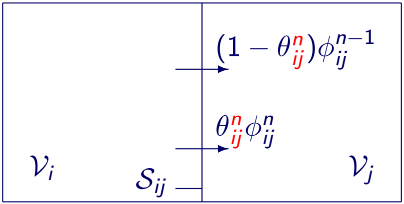
unstable
anti-diffusive
large Δt
small θ

The **grid** of Delft3D-WAQ is usually 3D, unstructured and **strongly non-uniform**



The idea is to minimize the numerical diffusion by choosing a **minimal local** $\theta_{ij}^{n} = \theta_{ji}^{n}$ **per flux**

$$\frac{|\mathcal{V}_i^n|\overline{c}_i^n - |\mathcal{V}_i^{n-1}|\overline{c}_i^{n-1}}{t_n - t_{n-1}} = -\sum_j |\mathcal{S}_{ij}^{n-1}|(1-\theta_{ij}^n)\phi_{ij}^{n-1} - \sum_j |\mathcal{S}_{ij}^n|\theta_{ij}^n\phi_{ij}^n$$



This is the creative idea of Mart Borsboom, one of my supervisors.

Assuming ‘conservation of water’, a **CFL-type condition** implies a local and a global maximum principle

$$|\mathcal{V}_i^{n-1}| - \Delta t_n \sum_j (1-\theta_{ij}^n)|\mathcal{S}_{ij}^{n-1}| \left(\max\{0, u_{ij}^{n-1}\} + \frac{\overline{\overline{d}}_{ij}^{n-1}}{\Delta x_{ij}} \right) \geq 0$$

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local maximum principle

Each concentration is a convex combination of the neighboring concentrations on which it depends.

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no spurious oscillations

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Each concentration lies between the minimum and maximum of the initial and the boundary conditions

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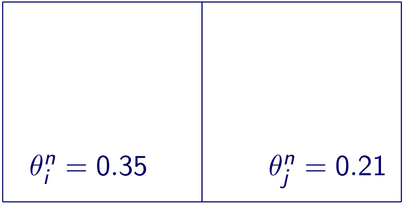
positivity preserving & L_∞-stability

A **practical choice** for θ_{ij}^n could be based on a value per grid cell

1. First, introduce an auxiliary coefficient θ_i^n for each grid cell:

$$\theta_i^n = \max\left\{0, 1 - \frac{|\mathcal{V}_i^{n-1}|}{\Delta t_n \sum_j |\mathcal{S}_{ij}^{n-1}| \left(\max\{0, u_{ij}^{n-1}\} + \frac{\bar{\bar{d}}_{ij}^{n-1}}{\|\underline{\mathbf{x}}_j^{n-1} - \underline{\mathbf{x}}_i^{n-1}\|_2}\right)}\right\}$$



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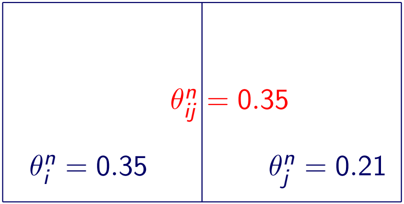
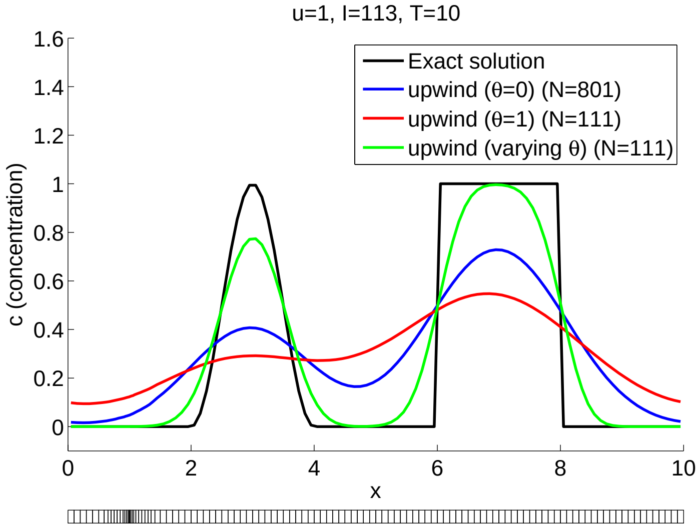
2. Finally, choose θ_{ij}^n as follows:

$$\theta_{ij} = \max\{\theta_i^n, \theta_j^n\}$$

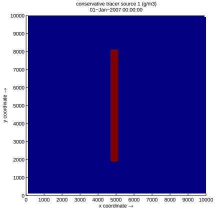


A varying minimal θ_{ij}^n leads to **less numerical diffusion** than $\theta = 1$

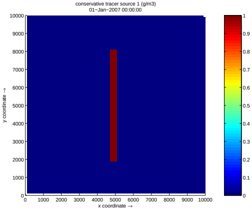


A varying minimal θ_{ij}^{n} leads to **less numerical diffusion** than $\theta = 1$

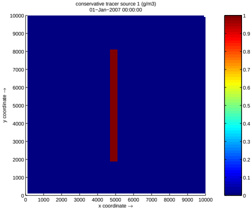
$\theta = 1$ ($\Delta t = 60\,\mathrm{s.}$)

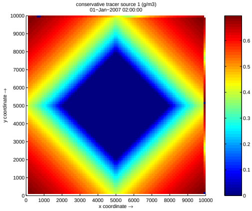


var. θ ($\Delta t = 60\,\mathrm{s.}$)

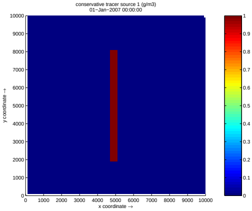


$\theta = 0$ ($\Delta t = 15\,\mathrm{s.}$)





var. θ coefficients



$\theta = 0$ & FCT

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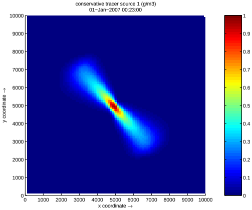

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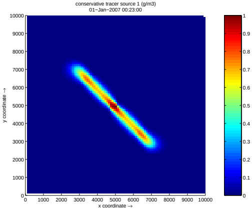

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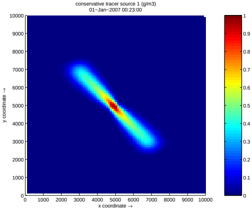

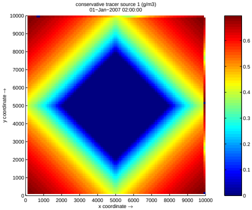

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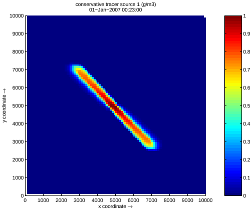

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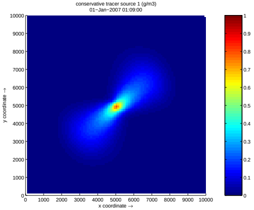

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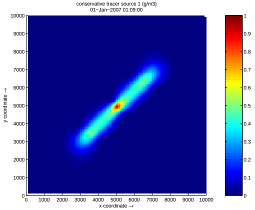

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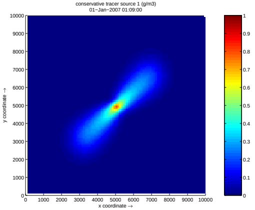

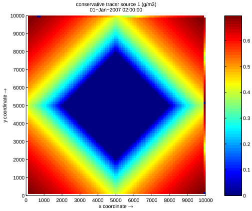

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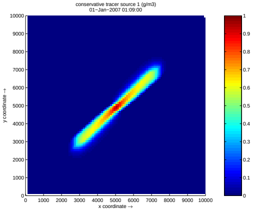

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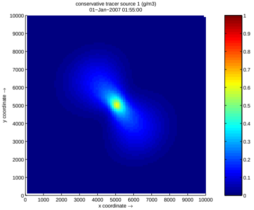

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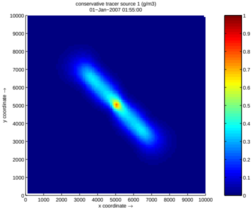

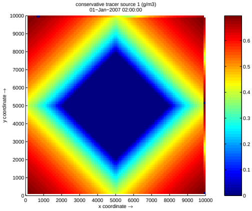

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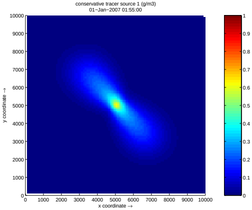

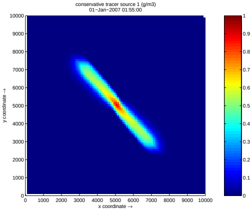

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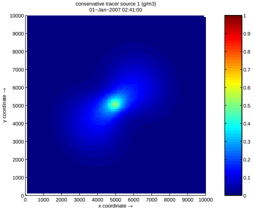

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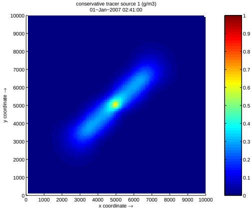

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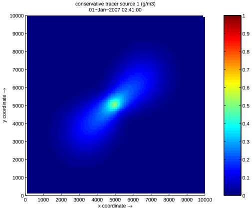

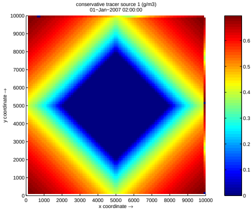

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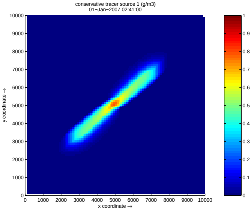

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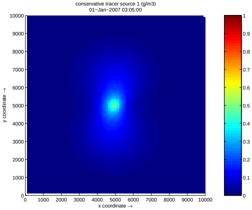
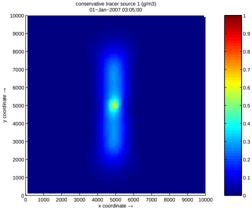
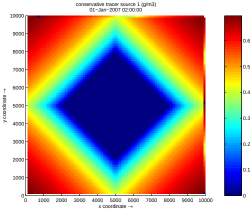


var. $\theta \; (\Delta t = 60\,\mathrm{s.})$





var. θ coefficients

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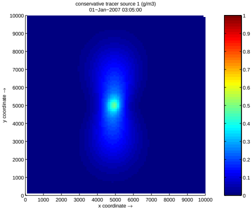
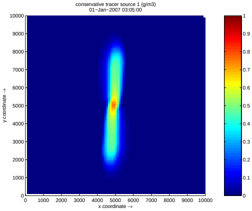
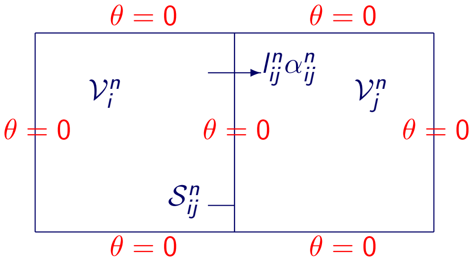




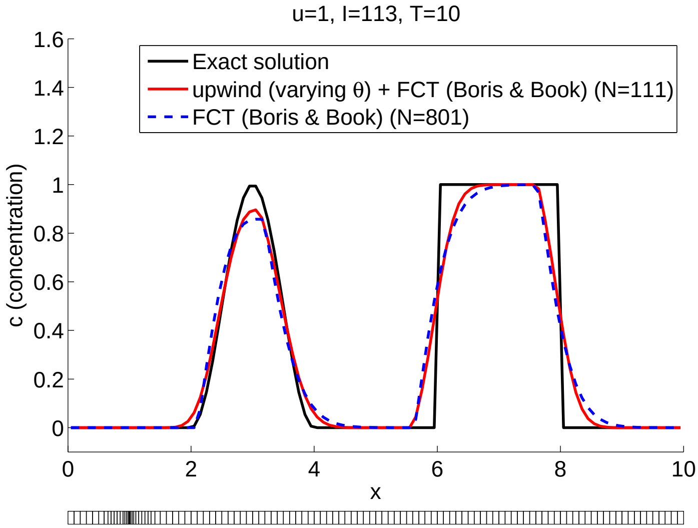
$\theta = 0$ & FCT

The variable-θ solution can be improved with a **higher order FCT approach** for 'explicit' edges

$$\overline{c}_i^n = \underbrace{\hat{\overline{c}}_i^n}_{\text{var. } \theta \text{ approx.}} - \Delta t_n \sum_{\text{'explicit' neighbours } j} |\mathcal{S}_{ij}^n| \underbrace{I_{ij}^n \alpha_{ij}^n}_{\text{limited flux corr.}}$$

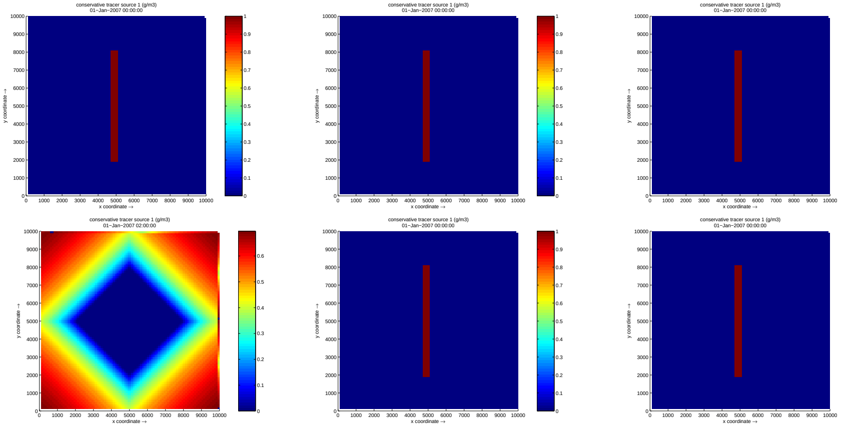


Updating the variable-θ solution with an FCT strategy leads to even **better accuracy**



Updating the variable-θ solution with an FCT strategy leads to even **better accuracy**

$\theta = 1$ ($\Delta t = 60\,\mathrm{s.}$) | var. θ ($\Delta t = 60\,\mathrm{s.}$) | $\theta = 0$ ($\Delta t = 15\,\mathrm{s.}$)



var. θ coefficients | var. θ & FCT | $\theta = 0$ & FCT

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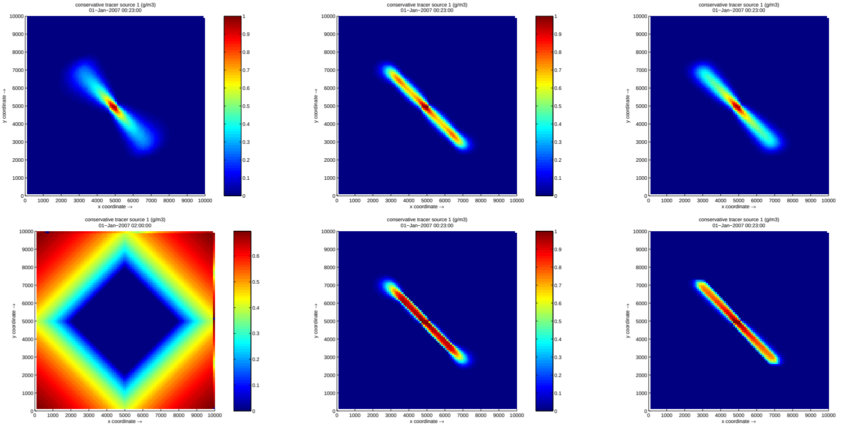

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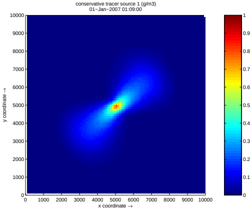
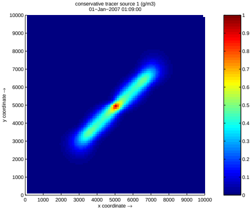
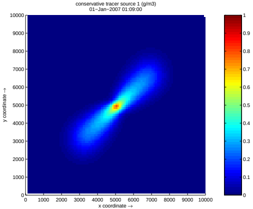
$\theta = 1$ ($\Delta t = 60\,\mathrm{s.}$)

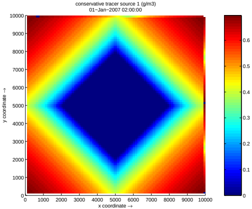


var. θ ($\Delta t = 60\,\mathrm{s.}$)

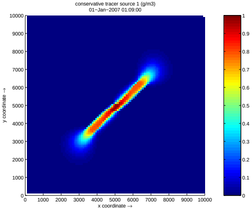


$\theta = 0$ ($\Delta t = 15\,\mathrm{s.}$)

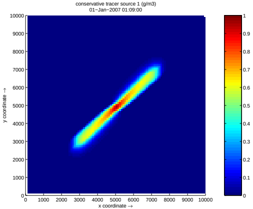




var. θ coefficients



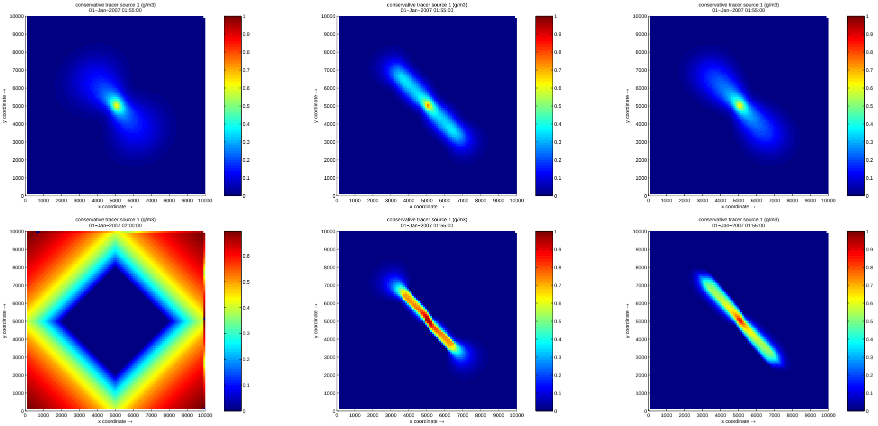
var. θ & FCT



$\theta = 0$ & FCT

Updating the variable-θ solution with an FCT strategy leads to even **better accuracy**

$\theta = 1$ ($\Delta t = 60\,\mathrm{s.}$) | var. θ ($\Delta t = 60\,\mathrm{s.}$) | $\theta = 0$ ($\Delta t = 15\,\mathrm{s.}$)



var. θ coefficients | var. θ & FCT | $\theta = 0$ & FCT

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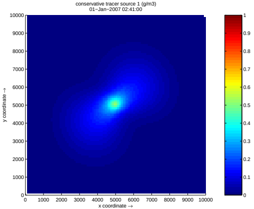
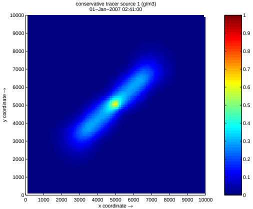
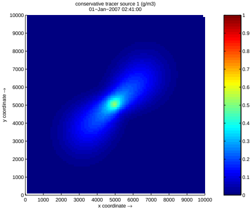
$\theta = 1$ ($\Delta t = 60\,\mathrm{s.}$)

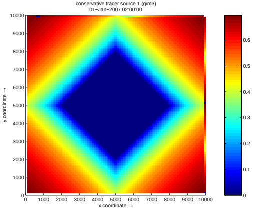


var. θ ($\Delta t = 60\,\mathrm{s.}$)

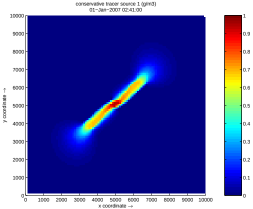


$\theta = 0$ ($\Delta t = 15\,\mathrm{s.}$)

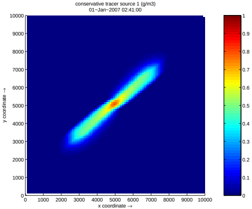




var. θ coefficients



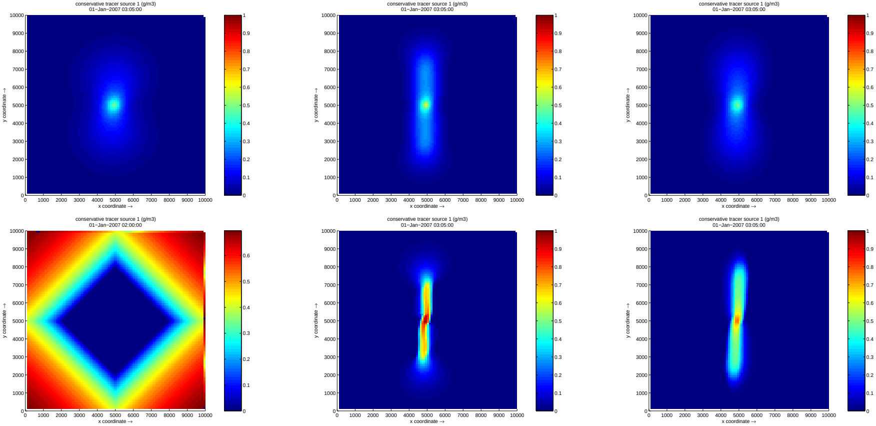
var. θ & FCT



$\theta = 0$ & FCT

Updating the variable-θ solution with an FCT strategy leads to even **better accuracy**

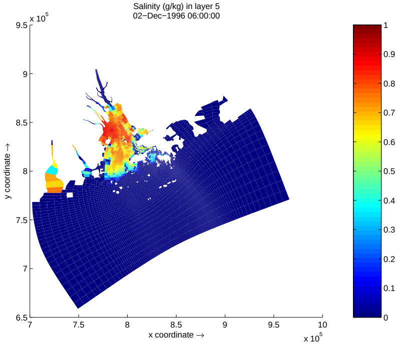
$\theta = 1$ ($\Delta t = 60\,\mathrm{s.}$) | var. θ ($\Delta t = 60\,\mathrm{s.}$) | $\theta = 0$ ($\Delta t = 15\,\mathrm{s.}$)



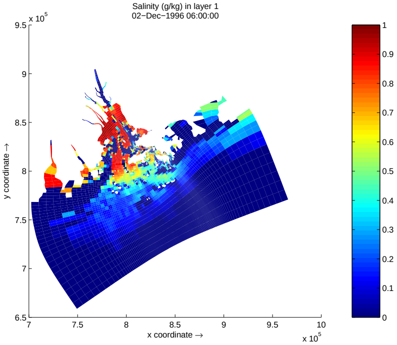
var. θ coefficients | var. θ & FCT | $\theta = 0$ & FCT

For the **Hong Kong model**, the **variable-θ coefficients** are larger in the surface layer than in the bottom layer

Bottom layer



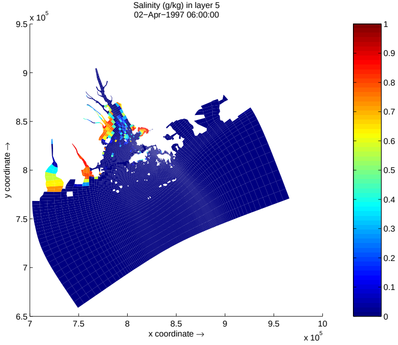
Surface layer



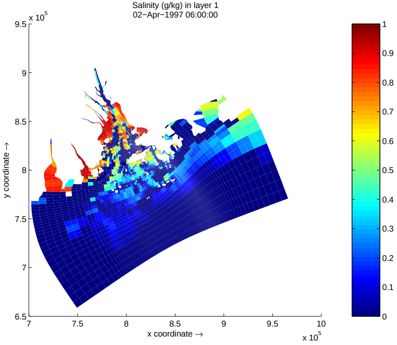
At the beginning of the simulation

For the **Hong Kong model**, the **variable-θ coefficients** are larger in the surface layer than in the bottom layer

Bottom layer



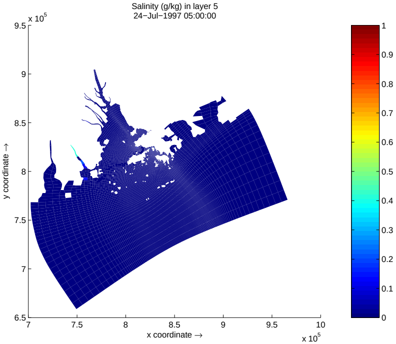
Surface layer



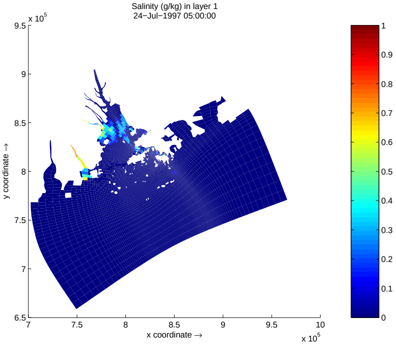
During the simulation

For the **Hong Kong model**, the **variable-θ coefficients** are larger in the surface layer than in the bottom layer

Bottom layer



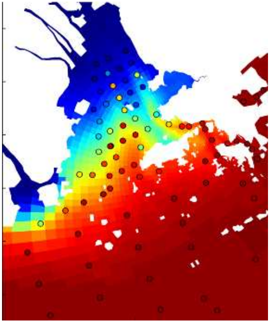
Surface layer



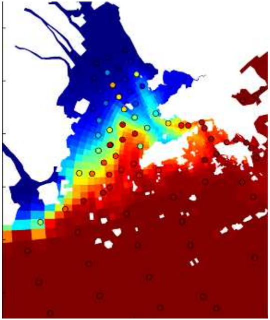
At the end of the simulation

For the **Hong Kong model**, the variable-θ FCT scheme performs well, compared to the existing schemes

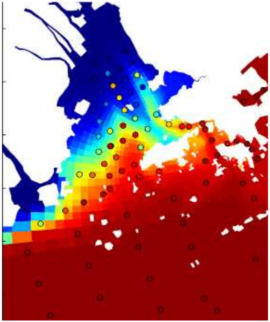
implict upwind
$\Delta t = 20\,\mathrm{min.}$
sim. time $= 20\,\mathrm{min.}$



variable-θ FCT
$\Delta t = 20\,\mathrm{min.}$
sim. time $= 29\,\mathrm{min.}$



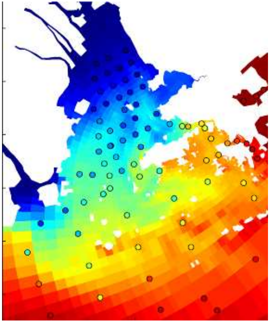
explicit FCT
$\Delta t = 1\,\mathrm{min.}$
sim. time $= 176\,\mathrm{min.}$



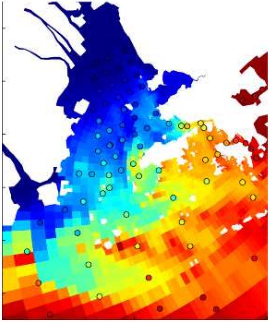
Bottom layer

For the **Hong Kong model**, the variable-θ FCT scheme performs well, compared to the existing schemes

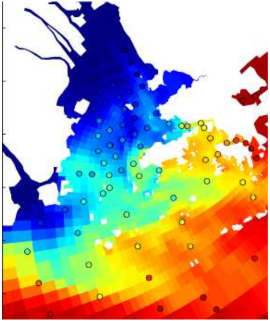
implict upwind
$\Delta t = 20\,\mathrm{min.}$
sim. time $= 20\,\mathrm{min.}$



variable-θ FCT
$\Delta t = 20\,\mathrm{min.}$
sim. time $= 29\,\mathrm{min.}$



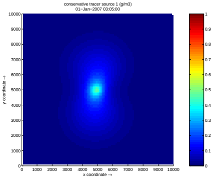
explicit FCT
$\Delta t = 1\,\mathrm{min.}$
sim. time $= 176\,\mathrm{min.}$

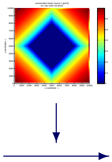


Surface layer

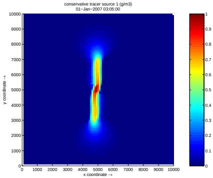
In **conclusion**, choosing θ variable seems a relevant step forwards towards a FVM that is **accurate and robust**

implicit upwind





variable-θ FCT



An iterative implicit FCT update, as proposed by Kuzmin et al., may lead to even better accuracy...

θhe End

Any questions or suggestions?