The following questions concern the mathematical verification of the 1D advection-dispersion-reaction solver, based on Strang Splitting which is basically developing for Sediment transport phenomenon in a tidal riverine network (flow can be, two way, highly advective or highly dispersive)

* Some Background on the method:





The equation to be solved is the above (mass conservation for constituent). The eq. 1 is the slave equation. A and U are provided by another solver which solves water's mass, and momentum equation in x direction for water. The schemes which are employed are as follows:

- Advection: Lax two step method (recast in FVM framework) please see the appendix.

-Dispersion: Crank-Nicolson time center (recast in FVM framework) please see the appendix.

-Reaction: Adaptive Runge-Kutta (RK-2,3)

* If I am to mathematically verify the equation (2) discretization, can I cancel out the A because it comes from another solver? does it have any impact on my verification? in other words should A and U for verification mission of equation (2), fulfill mass conservative of water [dQ/dx + dA/dt = 0].
* Is eq. (2) a linear equation if we neglect the non-linearity in Reaction term?
* I found two analytical solutions for advection dispersion equation in the following forms:





Do they need to be mass conservative for the mathematical verification mission?

Are they enough for my verification objective? or I still need to carry out method of manufactured solution or Richardson extrapolation to check K(x,t) and U(x,t)?

* Should I necessarily test the code with method of manufactured solution (MMS)? I think Richardson extrapolation also can be employed as an equivalent alternative. Does MMS provide any information which is not achievable with Richardson extrapolation?
* What is the practical measure of smoothness of a function? I run some tests and could not hit the nominal convergence "2", the convergence is around (1.7-1.8). The question is when can I blame smoothness of the solution to justify (1.7-1.8)? and when I should seek for other reasons (coding bug)?

The other point about smoothness of an initial mass distribution is that: if a test is run with an initial distribution with uniform flow and end up to an appropriate convergence ratio can I eliminate the smoothness issue from my check list in the tidal flow test with same mass distriution?

* Strang in his 1968 paper proved that if you have 2nd order operators and you assemble them in his recommended arrangement, the scheme will be 2nd order. [I know for practical reasons we cannot skip MMS or Richardson extrapolation]. The question is: Can I check each solver individually and the assembling procedure and then skip other verifications and refer to Strang and claim I have a 2nd order solver?
* Patrick Roache insists in his book and his paper on MMS[[1]](#footnote-1), you may pick any function for your manufactured solution and you should not worry about the fulfilling physics, the manufactured solution verification is 100% mathematical process. In the other words, if you just check the math your restrictions emerging from physics (e.g. negative concentration) shouldn't necessarily satisfy. Would you please give your opinion?

Answer By W. Kollmann

i can answer questions right now:  
(1) To check the accuracy of your equ. (2) you can cancel out the known field A, unless  
A is highly oscillatory. We don’t have a way of cancelling A  
(2) Equation (2) is linear for known A and linear source. We know that  
(3) You do not need to satisfy mass conservation for verification of (2). True in terms of verification, but you need it for the algorithm to work so there is no practical way of avoiding it. The dependence on  
the diffusivity K is only important if K depends strongly on x or t.   
(4)  Yes, you should check your code with MMS, since it allows you to see how the accuracy depends  
on the solution properties such as wavenumber/frequency range. Not if important relative scales are altered by an inappropriate choice of solution.  
(5) Smoothness measurement is tricky, you could use Fourier transform (if applicable) and check the  
spectral content. If the resolution is poor the sprectrum at the high wavenumber end is too large.  
Always assume a coding bug before you blame anything else. Your problem is not smoothness, it is a big mass conservation bug.  
(6) Yes  
(7) Roache is right. See above about relative scales. I do not see a way of avoiding this point.

**Appendix A-1: Advection, Lax Two Steps Method**

 (A1.1)

*A,Q,S*, and *Ks* are known from other parts:

*A* and *Q* from HYDRO

*Ks* from Diffusion

*S* (Sink and source come from decay, deposition and entrainment)

1- First half step:

 (A1.2)

Where









 (A1.3)

2- Second half step:

 (A1.4-a,b)

*x*

*t*

*n*

*n+½*

*n+1*

*i-1*

*i+1*

*i*

Figure A1: schematic of lax two step method

**Appendix A-2: Diffusion, Crank-Nicolson Method**



(A2.1)

 (A2.2)





is unknown in (A2.2) and other terms are known from measurements or previous step.



(A2.3)

In which *F* is diffusive flux re-writing (A3.2) yields:

 (A2.4)

1. **Neumann Boundary condition implementation**



Just by replacing F in the first and last diffusive flux Neumann Boundary condition will be implemented

* Middle row will be:



* First row: *i=1*



* Last row*: i=m*



1. * **Roache, P. J.**, (2002), *“Code Verification by the Method of Manufactured Solutions”*, J. of Fluid Eng., Vol. 124, pp. 4-10.

   **Roache, P. J.**, (2009), *“Fundamentals of Verification and Validation”*, Hermosa Publishers. [↑](#footnote-ref-1)