# VALIDATION OF THE PICS TRANSPORT CODE

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The PICS transport code [1], [2], [3] was validated using two different test problems with known analytic solutions. The first problem was a one-dimensional linear flood for a semi-infinite domain. An inflow (Dankwerts or Robin) boundary condition was imposed at the inflow end, and the initial concentration was taken to be zero. The problem under consideration was the following:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}, \qquad x > 0,\ t > 0, \tag{0.1}$$

$$uC - D\frac{\partial C}{\partial x} = uC^0, \qquad x = 0,\ t > 0. \tag{0.2}$$

Here, $C^0$ denotes the inflowing concentration, $D$ is the coefficient of dispersion, and $u$ denotes the velocity. The analytic solution of this problem is:

$$\begin{aligned} C(x,t) = {} & \operatorname{erfc}\left[\frac{x-t}{\sqrt{Dt}}\right] + \frac{t^{\frac{1}{2}}}{\pi D}\exp\left[-\frac{(x-t)^2}{4Dt}\right] \\ & + \frac{1}{2}\left[1 + \frac{x}{D} + \frac{t}{D}\right]\exp\left[\frac{x}{D}\right]\operatorname{erfc}\left[\frac{x+t}{2\sqrt{Dt}}\right]. \end{aligned}$$

For simplicity, we took $C^0 = 1$, $D = 0.01$, and $u = 1$.

The other test case was a three dimensional solution to the standard transport equation for one component, i.e.

$$\phi\frac{\partial C}{\partial t} - \nabla\cdot(D\nabla C - uC) = f, \tag{0.3}$$

where $\phi$ is the porosity. The domain of the problem was the unit cube, with an inflow boundary condition taken at the inflow face, where $x = 0$, and no dispersive flux specified at all other boundaries. A uniform initial concentration of 1 was prescribed. The hydrodynamic dispersion tensor was a multiple of the identity, $dI$, with $d = 0.01$. For simplicity, we took $\phi = 1$ and used a constant velocity field $u = (1, 0, 0)$. A concentration of the form

$$C(x,y,z,t) = te^{-t}x^2(1-x)^2\left[1 + y^2(1-y)^2 + z^2(1-z)^2\right] + 1 \tag{0.4}$$

satisfies the above transport equation with the given boundary and initial conditions and a distributed source function

$$\begin{aligned}
f(x,y,z,t) = {} & \phi\left(e^{-t} - te^{-t}\right)x^2(1-x)^2\left[1 + y^2(1-y)^2 + z^2(1-z)^2\right] \\
& + \left[2x(1-x)^2 - 2x^2(1-x)\right]te^{-t}\left[1 + y^2(1-y)^2 + z^2(1-z)^2\right] \\
& - dte^{-t}\left[2(1-x)^2 - 8x(1-x) + 2x^2\right]\left[1 + y^2(1-y)^2 + z^2(1-z)^2\right] \\
& - dte^{-t}x^2(1-x)^2\Big[2(1-y)^2 - 8y(1-y) \\
& \qquad + 2y^2 + 2(1-z)^2 - 8z(1-z) + 2z^2\Big].
\end{aligned}$$

For both test cases, we approximated the equations up to $t = 0.5\,\mathrm{PVI}$ (pore volume injected). In the one dimensional case, which assumes a semi-infinite domain, it was verified that the solution had not come into contact with the outflow boundary at this time.

Convergence results were tabulated for both problems. The error is the difference between the true and computed solutions, and it was measured in the $\ell_\infty(L_2)$-norm. This norm is given by maximizing the spatial $L_2$-norm over the taken time steps. The $L_2$-norm was approximated with the midpoint rule of integration. Theoretical results [2] show that the convergence rate is at least

$$\text{error} \le C\,(h^{1.5} + \Delta t), \tag{0.5}$$

where $\Delta t$ is the time step size and $h$ is the grid spacing. We believe that the spatial convergence rate is actually 2, not 1.5, so we took in all cases $\Delta t$ proportional to $h^2$. Our results determine the spatial convergence rate.

As can be seen in Table 1, the three dimensional problem exhibited a quadratic rate of convergence (linear regression gives the rate as 2.1179). For the one dimensional problem, the rate was approximated by considering the error at time steps away from the initial condition (Table 2) and also, in a separate series of runs, at the final time step only (Table 3). The measured rate in the former case was 1.4667, while in the latter case, a quadratic rate was observed (2.0003). The lower rate in the former case may be due to the sharp front which the solution exhibits at early time.

Table 1. Approximation errors for the three dimensional example.

| Number of elements | Time step size (PVI) | Maximum $L_2$-error | Number of Processors | Time in transport |
|---|---|---|---|---|
| 5×5×5 | 0.1000 | 0.004626 | 1×1×1 | 58.585 |
| 10×10×10 | 0.0250 | 0.001102 | 2×2×1 | 490.785 |
| 15×15×15 | 0.0111 | 0.000459 | 4×2×1 | 2124.502 |
| 20×20×20 | 0.0063 | 0.000248 | 4×2×1 | 8061.628 |
| 40×40×40 | 0.0016 | 0.000057 | 4×4×1 | 126625.947 |

Table 2. Approximation errors for the one dimensional example.

| Number of elements | Time step size (PVI) | Maximum $L_2$-error |
|---|---|---|
| 10 | 0.10000 | 0.032453 |
| 20 | 0.02500 | 0.013409 |
| 40 | 0.00630 | 0.005248 |
| 80 | 0.00160 | 0.001202 |
| 160 | 0.00037 | 0.000672 |

Table 3. Approximation errors for the one dimensional example, at the final time.

| Number of elements | Time step size (PVI) | Final $L_2$-error |
|---|---|---|
| 10 | 0.10000 | 0.024189 |
| 20 | 0.02500 | 0.009043 |
| 40 | 0.00630 | 0.003153 |
| 60 | 0.00280 | 0.001450 |
| 80 | 0.00160 | 0.000801 |
| 120 | 0.00069 | 0.000351 |
| 160 | 0.00037 | 0.000200 |

A plot of the concentration profile of the one dimensional solution at 0.25 PVI and 0.5 PVI is shown in Figure 1, for the 40 element computation. It clearly shows a superb match between the approximate and analytic solutions. Figure 2 shows the one dimensional solution with zero dispersion ($D = 0$), a time step of 0.025 PVI, and 40 and 80 elements. As can be seen, the amount of numerical dispersion is quite small.

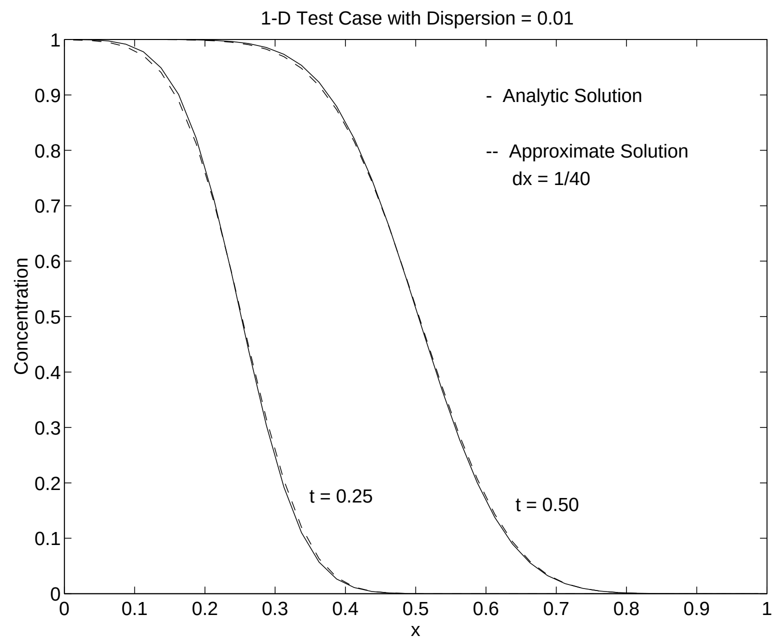


Fig. 1. Concentration profile of the one dimensional solution.

Parallel speed-ups curves were calculated for the three dimensional problem. These curves show the ratio of the run time on one processor divided by the run time on $n$ processors. A perfectly parallel computation will have linear speed-up; that is, the run time for $n$ processors will be $n$ times faster than on one processor. The speed-ups are shown in Figure 3 for a $16\times16\times16$ and a $24\times24\times24$ spatial discretization. The curves are nearly linear.

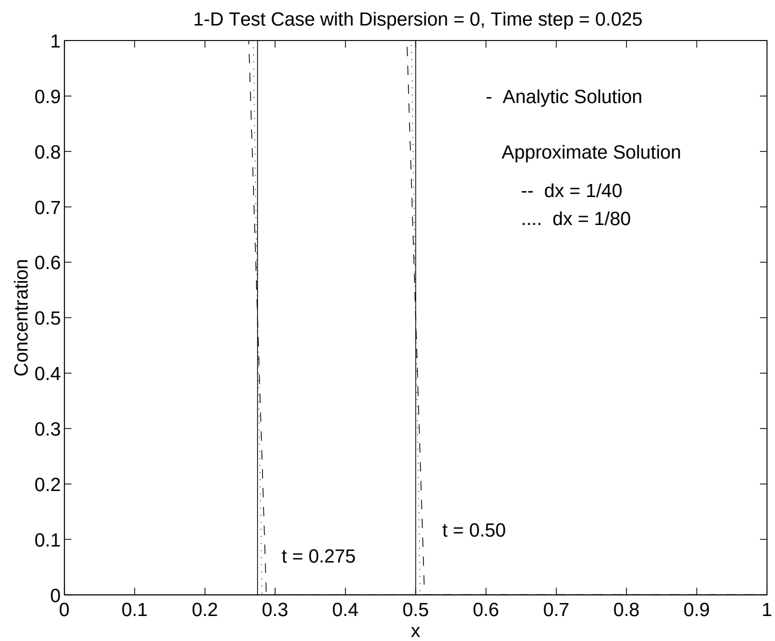

Fig. 2. Concentration profile of the one dimensional solution with no physical dispersion.

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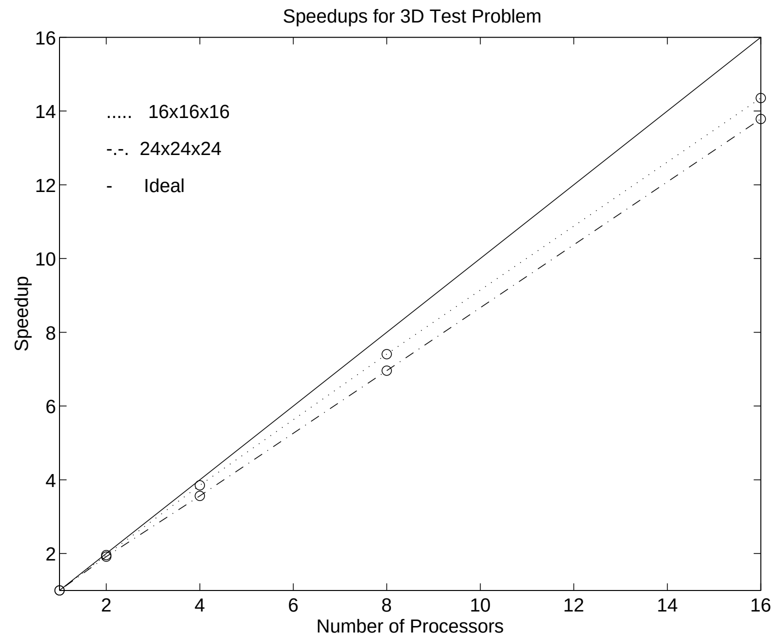


Fig. 3. Parallel speed-up curves.

## References


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