

TECHNICAL REPORT

ShockTube Problem - Status Report 1 Uni-Level Experiments

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Abstract:

We describe the research development on the shock tube problem. We tested SUS with a single level (no AMR), for various parameter sets, to conclude on ICEs accuracy with a uniform, non-composite grid. The report is chronological and describes the problems encountered, and their resolution.

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We describe the research development on the shock tube problem. We tested SUS with a single level (no AMR), for various parameter sets, to conclude on ICE's accuracy with a uniform, non-composite grid. The report is chronological and describes the problems encountered, and their resolution.

Key words. ICE, SUS, time-stepping CFD codes, numerical experiments.

1 Goals

Our goal is to understand the behaviour of the ICE code with one level (a uniform grid extending over the full domain, as it was used prior to Todd's work). More specifically, we study

1. The spatial order of accuracy, by varying $h \equiv \Delta x$.
2. The temporal order of accuracy, by varying Δt .
3. The behaviour of a first-order versus a second-order advection operator, near and away from discontinuities (in pressure, temperature, etc., that is, shocks).

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2 Indicators

To check the accuracy of our numerical solutions, our standard test is running ICE on a series of increasingly finer grids. For each grid (i.e. for each meshsize h , or number of cells N in the x -direction; note that this is effectively a 1D problem, so space includes only the x -variable) we compute the difference (error) between the numerical solution and the exact solution, which was obtained using Todd's *Numerica* code, at the final simulation time.

Because of the dynamic timestep size, the final simulation times are slightly different for different h 's. Albeit, they were still similar to each other, because our target simulation time was $t = .0005[s]$ for all runs, the final simulation time being the last discrete time hit before t was reached.

For each function (p, T, u, ρ , where u is the velocity in the x -direction), we computed the global relative errors

$$\varepsilon^h := \frac{\|u^h - U^h\|_p}{\|U^h\|_p}, \quad (1)$$

where $\|\cdot\|_p$ is the discrete scaled spatial l_p norm of a function defined on grid h , namely,

$$\|u\|_p := \left(\frac{1}{N} \sum_{i=1}^N |u_i|^p \right)^{\frac{1}{p}}, \quad N := \text{number of cells}, \quad (2)$$

U is the exact solution, U^h is the exact solution evaluated at the grid- h cells (mid-points), and u^h is the numerical solution obtained at grid h . We used both $p = 1, 2$, so that when the ratio of l_2 to l_1 error norm is large, it indicates that large errors are concentrated in "narrow regions", most probably, around shocks.

Finally, we compute the estimated order α of algebraic convergence of the numerical solutions to the exact one. Namely, we assume the error is a power law of the meshsize, $\varepsilon = Ch^\alpha$. The exponent is estimated by comparing three grids,

$$\text{alpha} = \log_2 \left(\frac{\varepsilon^{2h}}{\varepsilon^h} \right), \quad (3)$$

for a sufficiently fine h (we used $N = 1600$ as the h -grid here).

In addition, we plot the exact solution, numerical solution and the error in u , to get a visual confirmation of the global numbers.

2.1 Software Flow

In producing the results, we used the following steps to obtain the results for a given parameter sets, employing automated scripts:

- Initialization of directory structure: each run “type” (a certain set of parameters) is assigned a parent directory, under which different directories contain the different resolutions (100, 200, . . . cells). Within each directory, we store the standard UDA output directory, and our outputs (including the exact solution data). We start by creating the UPS input files in each of these directories.
- SUS is then run in each of these directories, with the corresponding UPS files [inferno].
- Post-processing includes computing the final time and time step of the simulation, and computing the exact solution at this time [SGI, e.g., rapture].
- A MATLAB scripts takes the post-processed data and produces plots and statistics on the numerical accuracy at different resolutions. The output is written to EPS figure files, and a \LaTeX main results file.
- The result files are embedded within this report.

3 Spatial Error, Original Parameters

First, we used the default parameter set in the UPS file. The important features were:

- Time steps controlled by CFL = .45.
- Second order advection operator.
- All (including MPM source terms) were “turned on” (this is in fact not sure; need to check with Todd).

Table 1: Original parameters: relative l_1 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
100	78	$4.9964 \cdot 10^{-4}$	$2.02 \cdot 10^{-2}$	$6.72 \cdot 10^{-2}$	$2.14 \cdot 10^{-2}$	$1.86 \cdot 10^{-2}$
200	158	$4.9960 \cdot 10^{-4}$	$1.25 \cdot 10^{-2}$	$4.20 \cdot 10^{-2}$	$1.27 \cdot 10^{-2}$	$1.38 \cdot 10^{-2}$
400	318	$4.9951 \cdot 10^{-4}$	$8.02 \cdot 10^{-3}$	$2.97 \cdot 10^{-2}$	$8.16 \cdot 10^{-3}$	$1.04 \cdot 10^{-2}$
800	638	$4.9952 \cdot 10^{-4}$	$5.32 \cdot 10^{-3}$	$2.03 \cdot 10^{-2}$	$5.23 \cdot 10^{-3}$	$8.38 \cdot 10^{-3}$
1600	1279	$4.9984 \cdot 10^{-4}$	$3.92 \cdot 10^{-3}$	$1.66 \cdot 10^{-2}$	$3.82 \cdot 10^{-3}$	$7.50 \cdot 10^{-3}$
Estimated Order			0.4413	0.2887	0.4518	0.1592

Table 2: Original parameters: relative l_2 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
100	78	$4.9964 \cdot 10^{-4}$	$3.19 \cdot 10^{-2}$	$1.27 \cdot 10^{-1}$	$3.80 \cdot 10^{-2}$	$5.69 \cdot 10^{-2}$
200	158	$4.9960 \cdot 10^{-4}$	$2.33 \cdot 10^{-2}$	$1.15 \cdot 10^{-1}$	$2.83 \cdot 10^{-2}$	$5.00 \cdot 10^{-2}$
400	318	$4.9951 \cdot 10^{-4}$	$1.76 \cdot 10^{-2}$	$1.15 \cdot 10^{-1}$	$2.36 \cdot 10^{-2}$	$3.96 \cdot 10^{-2}$
800	638	$4.9952 \cdot 10^{-4}$	$1.38 \cdot 10^{-2}$	$1.01 \cdot 10^{-1}$	$1.91 \cdot 10^{-2}$	$3.42 \cdot 10^{-2}$
1600	1279	$4.9984 \cdot 10^{-4}$	$1.22 \cdot 10^{-2}$	$1.00 \cdot 10^{-1}$	$1.77 \cdot 10^{-2}$	$3.23 \cdot 10^{-2}$
Estimated Order			0.1798	0.0138	0.1063	0.0826

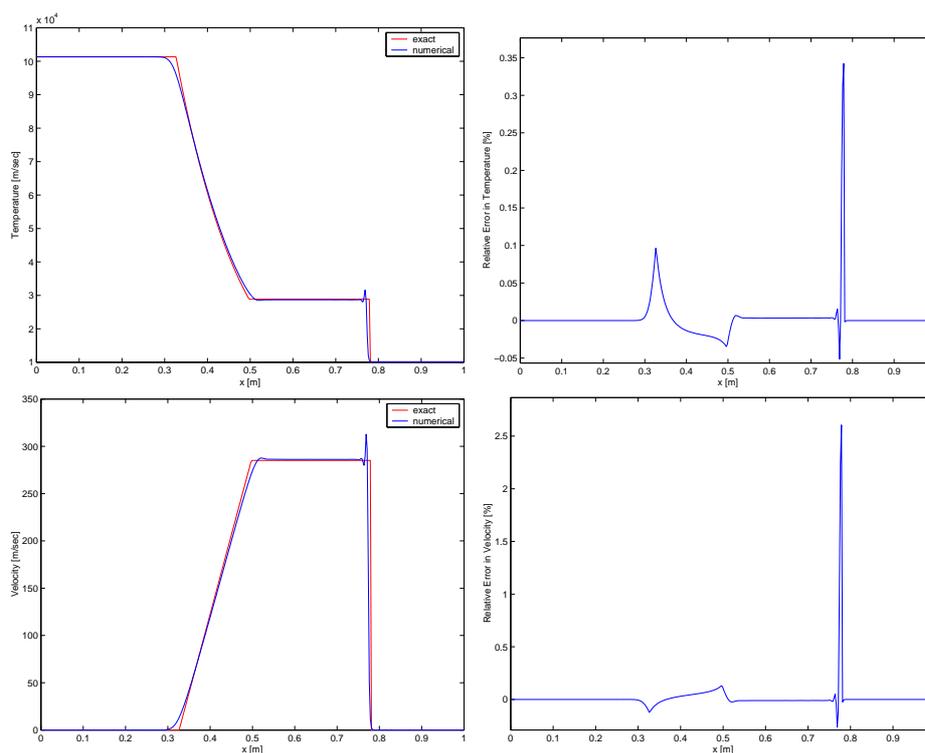


Figure 1: Original parameters: Upper row: temperature; lower row: velocity. Left: exact vs. numerical solution for $N = 1600$, at the final simulation time. Right: relative error in the velocity.

4 Spatial Error, CFL = .05, Second-Order Advection

The results in §3 contain both the spatial and temporal errors. To eliminate the latter, we repeat the results with a smaller timestep, controlled by CFL = .05 instead of CFL = .45.

Table 3: Small CFL, Second order advection: relative l_1 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
100	720	$4.9954 \cdot 10^{-4}$	$1.70 \cdot 10^{-2}$	$6.00 \cdot 10^{-2}$	$1.76 \cdot 10^{-2}$	$1.71 \cdot 10^{-2}$
200	1459	$4.9991 \cdot 10^{-4}$	$9.86 \cdot 10^{-3}$	$3.60 \cdot 10^{-2}$	$9.94 \cdot 10^{-3}$	$1.09 \cdot 10^{-2}$
400	2940	$4.9990 \cdot 10^{-4}$	$6.08 \cdot 10^{-3}$	$2.42 \cdot 10^{-2}$	$6.04 \cdot 10^{-3}$	$8.87 \cdot 10^{-3}$
800	5902	$4.9997 \cdot 10^{-4}$	$3.93 \cdot 10^{-3}$	$1.53 \cdot 10^{-2}$	$3.61 \cdot 10^{-3}$	$7.03 \cdot 10^{-3}$
1600	11825	$4.9997 \cdot 10^{-4}$	$2.91 \cdot 10^{-3}$	$1.25 \cdot 10^{-2}$	$2.64 \cdot 10^{-3}$	$6.28 \cdot 10^{-3}$
Estimated Order			0.4334	0.2820	0.4534	0.1624

Table 4: Small CFL, Second order advection: relative l_2 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
100	720	$4.9954 \cdot 10^{-4}$	$2.76 \cdot 10^{-2}$	$1.17 \cdot 10^{-1}$	$3.09 \cdot 10^{-2}$	$5.66 \cdot 10^{-2}$
200	1459	$4.9991 \cdot 10^{-4}$	$2.02 \cdot 10^{-2}$	$1.07 \cdot 10^{-1}$	$2.33 \cdot 10^{-2}$	$3.98 \cdot 10^{-2}$
400	2940	$4.9990 \cdot 10^{-4}$	$1.57 \cdot 10^{-2}$	$1.04 \cdot 10^{-1}$	$1.99 \cdot 10^{-2}$	$3.83 \cdot 10^{-2}$
800	5902	$4.9997 \cdot 10^{-4}$	$1.24 \cdot 10^{-2}$	$8.65 \cdot 10^{-2}$	$1.57 \cdot 10^{-2}$	$3.23 \cdot 10^{-2}$
1600	11825	$4.9997 \cdot 10^{-4}$	$1.11 \cdot 10^{-2}$	$8.78 \cdot 10^{-2}$	$1.52 \cdot 10^{-2}$	$3.01 \cdot 10^{-2}$
Estimated Order			0.1511	-0.0206	0.0477	0.1012

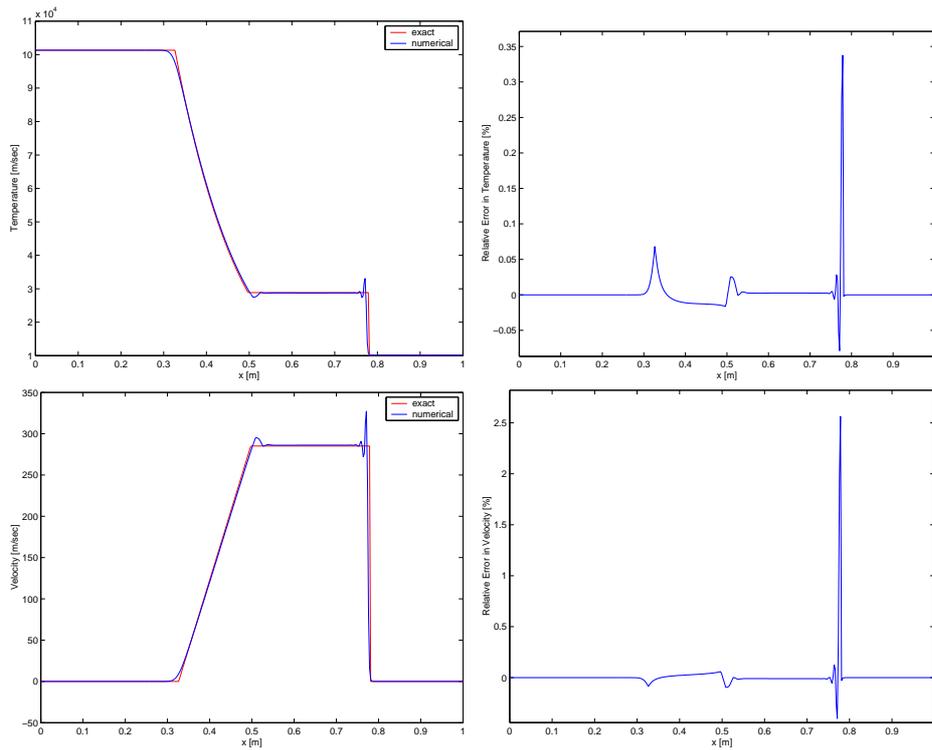


Figure 2: Small CFL, Second order advection: Upper row: temperature; lower row: velocity. Left: exact vs. numerical solution for $N = 1600$, at the final simulation time. Right: relative error in the velocity.

5 Spatial Error, CFL = .05, First-Order Advection

We repeat the results of §4 with a spatial first-order advection operator, which is expected to produce more accurate results near the shock locations. Again, to minimize temporal errors, we use a timestep controlled by CFL = .05.

Table 5: Small CFL, First order advection: relative l_1 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
100	672	$4.9945 \cdot 10^{-4}$	$2.61 \cdot 10^{-2}$	$6.48 \cdot 10^{-2}$	$2.03 \cdot 10^{-2}$	$3.26 \cdot 10^{-2}$
200	1381	$4.9967 \cdot 10^{-4}$	$1.75 \cdot 10^{-2}$	$3.93 \cdot 10^{-2}$	$1.25 \cdot 10^{-2}$	$2.39 \cdot 10^{-2}$
400	2799	$4.9991 \cdot 10^{-4}$	$1.20 \cdot 10^{-2}$	$2.68 \cdot 10^{-2}$	$8.04 \cdot 10^{-3}$	$1.76 \cdot 10^{-2}$
800	5635	$4.9996 \cdot 10^{-4}$	$8.19 \cdot 10^{-3}$	$1.75 \cdot 10^{-2}$	$5.05 \cdot 10^{-3}$	$1.33 \cdot 10^{-2}$
1600	11309	$4.9999 \cdot 10^{-4}$	$5.86 \cdot 10^{-3}$	$1.40 \cdot 10^{-2}$	$3.53 \cdot 10^{-3}$	$1.06 \cdot 10^{-2}$
Estimated Order			0.4819	0.3234	0.5157	0.3185

Table 6: Small CFL, First order advection: relative l_2 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
100	672	$4.9945 \cdot 10^{-4}$	$3.90 \cdot 10^{-2}$	$1.12 \cdot 10^{-1}$	$3.53 \cdot 10^{-2}$	$7.83 \cdot 10^{-2}$
200	1381	$4.9967 \cdot 10^{-4}$	$3.04 \cdot 10^{-2}$	$9.58 \cdot 10^{-2}$	$2.57 \cdot 10^{-2}$	$6.82 \cdot 10^{-2}$
400	2799	$4.9991 \cdot 10^{-4}$	$2.47 \cdot 10^{-2}$	$9.53 \cdot 10^{-2}$	$2.08 \cdot 10^{-2}$	$5.74 \cdot 10^{-2}$
800	5635	$4.9996 \cdot 10^{-4}$	$2.00 \cdot 10^{-2}$	$8.07 \cdot 10^{-2}$	$1.60 \cdot 10^{-2}$	$4.92 \cdot 10^{-2}$
1600	11309	$4.9999 \cdot 10^{-4}$	$1.71 \cdot 10^{-2}$	$8.41 \cdot 10^{-2}$	$1.51 \cdot 10^{-2}$	$4.37 \cdot 10^{-2}$
Estimated Order			0.2300	-0.0589	0.0850	0.1709

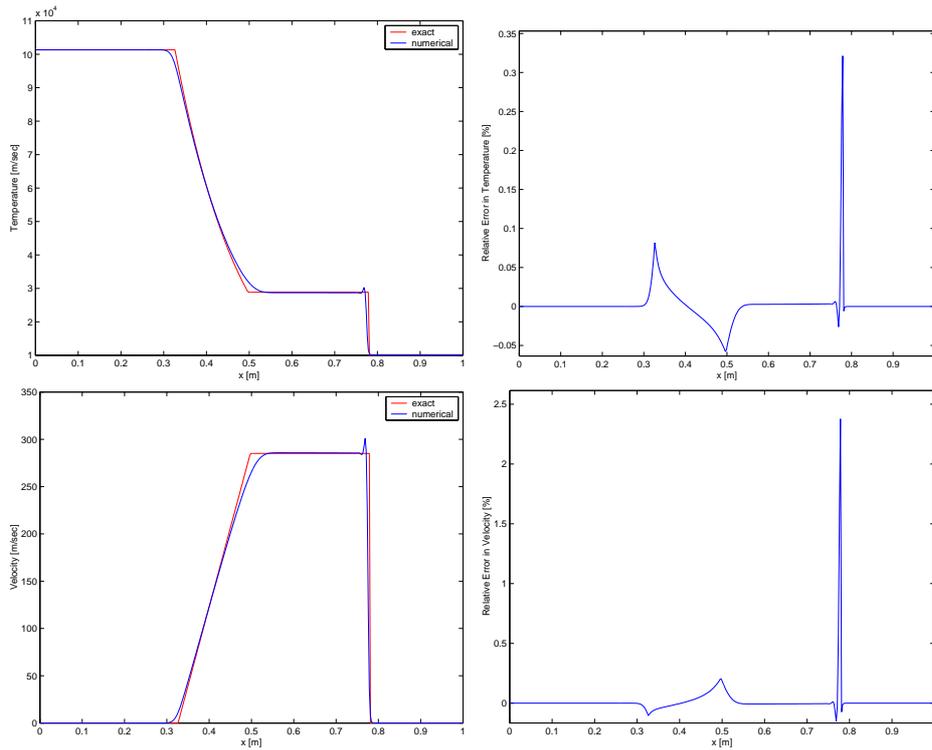


Figure 3: Small CFL, First order advection: Upper row: temperature; lower row: velocity. Left: exact vs. numerical solution for $N = 1600$, at the final simulation time. Right: relative error in the velocity.

6 Temporal Error, $N = 800$, Second-Order Advection

Here we study the numerical accuracy versus Δt . In fact, we can control Δt 's size only indirectly, through the CFL number. We tested a series of increasingly smaller CFL's on a sufficiently fine spatial grid ($N = 800$), so that spatial errors should not dominate the overall accuracy.

Table 7: Dependence on timestep size, Second order advection: relative l_1 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
040	720	$4.9949 \cdot 10^{-4}$	$5.14 \cdot 10^{-3}$	$1.98 \cdot 10^{-2}$	$5.03 \cdot 10^{-3}$	$8.22 \cdot 10^{-3}$
020	1460	$4.9989 \cdot 10^{-4}$	$4.37 \cdot 10^{-3}$	$1.69 \cdot 10^{-2}$	$4.17 \cdot 10^{-3}$	$7.54 \cdot 10^{-3}$
010	2940	$4.9985 \cdot 10^{-4}$	$4.06 \cdot 10^{-3}$	$1.58 \cdot 10^{-2}$	$3.78 \cdot 10^{-3}$	$7.21 \cdot 10^{-3}$
005	5902	$4.9997 \cdot 10^{-4}$	$3.93 \cdot 10^{-3}$	$1.53 \cdot 10^{-2}$	$3.61 \cdot 10^{-3}$	$7.03 \cdot 10^{-3}$
Estimated Order			0.0472	0.0485	0.0664	0.0381

Table 8: Dependence on timestep size, Second order advection: relative l_2 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
040	720	$4.9949 \cdot 10^{-4}$	$1.36 \cdot 10^{-2}$	$1.00 \cdot 10^{-1}$	$1.88 \cdot 10^{-2}$	$3.40 \cdot 10^{-2}$
020	1460	$4.9989 \cdot 10^{-4}$	$1.28 \cdot 10^{-2}$	$9.19 \cdot 10^{-2}$	$1.69 \cdot 10^{-2}$	$3.31 \cdot 10^{-2}$
010	2940	$4.9985 \cdot 10^{-4}$	$1.25 \cdot 10^{-2}$	$8.92 \cdot 10^{-2}$	$1.62 \cdot 10^{-2}$	$3.26 \cdot 10^{-2}$
005	5902	$4.9997 \cdot 10^{-4}$	$1.24 \cdot 10^{-2}$	$8.65 \cdot 10^{-2}$	$1.57 \cdot 10^{-2}$	$3.23 \cdot 10^{-2}$
Estimated Order			0.0200	0.0446	0.0469	0.0151

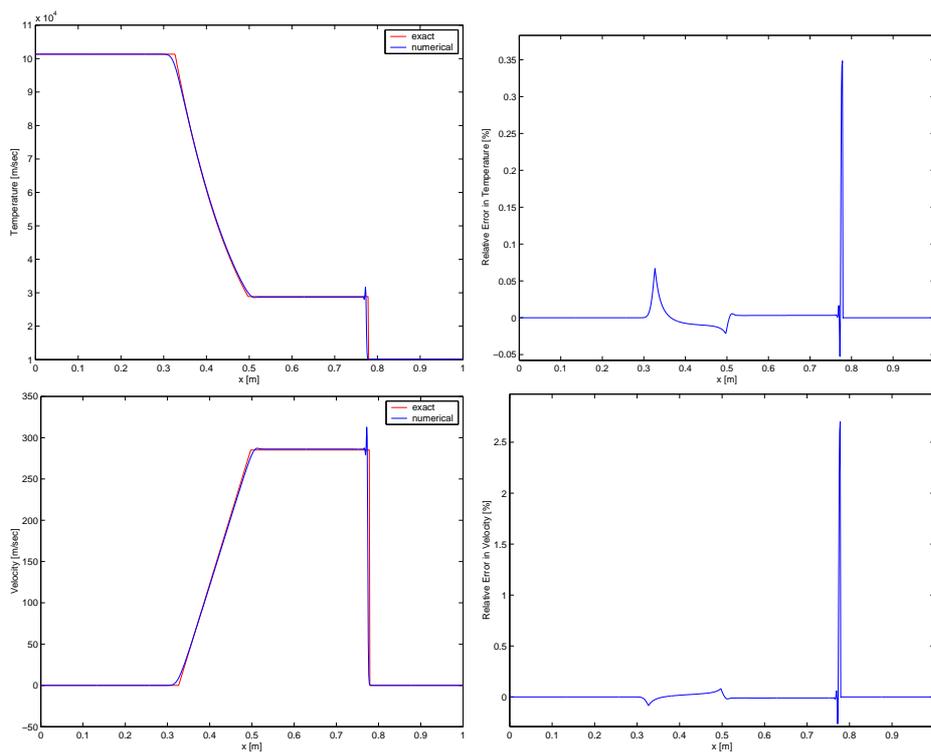


Figure 4: Dependence on timestep size, Second order advection: Upper row: temperature; lower row: velocity. Left: exact vs. numerical solution for $N = 1600$, at the final simulation time. Right: relative error in the velocity.

7 Temporal Error, $N = 800$, First-Order Advection

Here we study the numerical accuracy versus Δt as in §6, but this time we use a first-order advection operator.

Table 9: Dependence on timestep size, First order advection: relative l_1 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
040	694	$4.9959 \cdot 10^{-4}$	$8.98 \cdot 10^{-3}$	$2.10 \cdot 10^{-2}$	$6.37 \cdot 10^{-3}$	$1.35 \cdot 10^{-2}$
020	1399	$4.9987 \cdot 10^{-4}$	$8.52 \cdot 10^{-3}$	$1.89 \cdot 10^{-2}$	$5.59 \cdot 10^{-3}$	$1.34 \cdot 10^{-2}$
010	2811	$4.9998 \cdot 10^{-4}$	$8.29 \cdot 10^{-3}$	$1.79 \cdot 10^{-2}$	$5.22 \cdot 10^{-3}$	$1.33 \cdot 10^{-2}$
005	5635	$4.9996 \cdot 10^{-4}$	$8.19 \cdot 10^{-3}$	$1.75 \cdot 10^{-2}$	$5.05 \cdot 10^{-3}$	$1.33 \cdot 10^{-2}$
Estimated Order			0.0181	0.0312	0.0471	0.0030

Table 10: Dependence on timestep size, First order advection: relative l_2 error norms

N	Final Timestep	Final Time [s]	p	T	u	ρ
040	694	$4.9959 \cdot 10^{-4}$	$2.04 \cdot 10^{-2}$	$8.80 \cdot 10^{-2}$	$1.85 \cdot 10^{-2}$	$4.85 \cdot 10^{-2}$
020	1399	$4.9987 \cdot 10^{-4}$	$2.02 \cdot 10^{-2}$	$8.34 \cdot 10^{-2}$	$1.71 \cdot 10^{-2}$	$4.89 \cdot 10^{-2}$
010	2811	$4.9998 \cdot 10^{-4}$	$2.01 \cdot 10^{-2}$	$8.12 \cdot 10^{-2}$	$1.63 \cdot 10^{-2}$	$4.91 \cdot 10^{-2}$
005	5635	$4.9996 \cdot 10^{-4}$	$2.00 \cdot 10^{-2}$	$8.07 \cdot 10^{-2}$	$1.60 \cdot 10^{-2}$	$4.92 \cdot 10^{-2}$
Estimated Order			0.0022	0.0086	0.0244	-0.0031

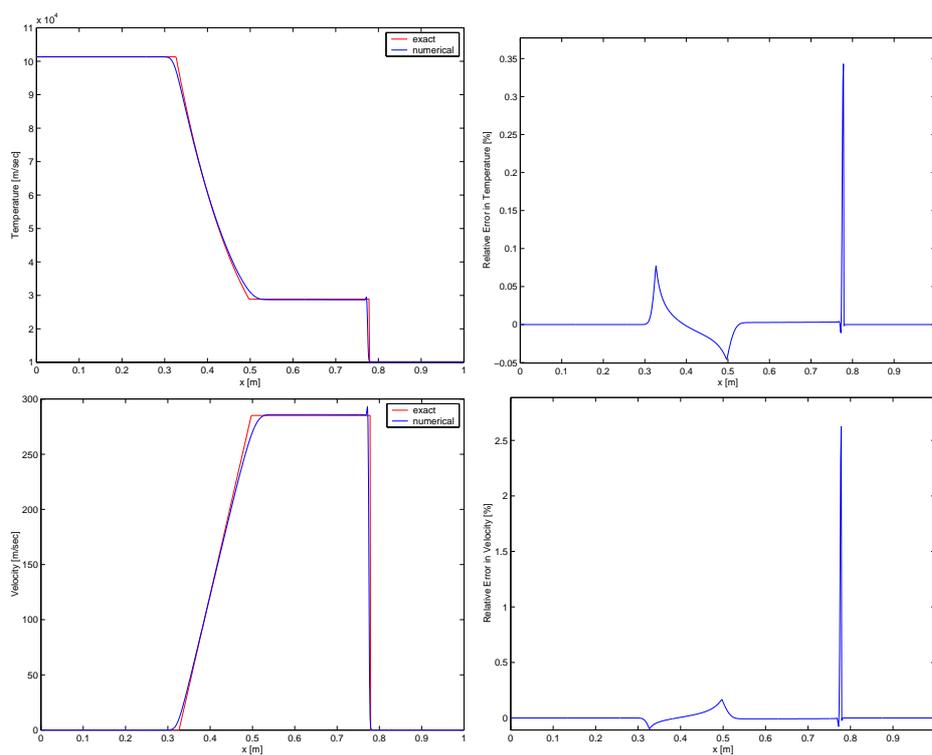


Figure 5: Dependence on timestep size, First order advection: Upper row: temperature; lower row: velocity. Left: exact vs. numerical solution for $N = 1600$, at the final simulation time. Right: relative error in the velocity.

8 Conclusions

We examined ICE's numerical solution accuracy versus an exact solution for a model problem. We investigated the behaviour of the numerical error versus different parameters (h , Δt , order of advection).

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- ...