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NA 620 – HW 2

**Question 1 – Scheme Comparison**

The OpenFOAM command, scalarTransportFoam, was used to solve *Equation 1*, seen below.

*Eqn. 1*

*Figures 1-4* show the solution to this equation using the discretization schemes of linear, linear upwind, upwind, and van Leer plotted on one structured grid and three unstructured grids of three varying coarsenesses.

*Figure 1 – Four Discretization Schemes on 20 x 20 Structured Grid*

*Figure 2 – Three Discretization Schemes on 20 x 20 Unstructured Grid*

*Figure 3 – Three Discretization Schemes on 40 x 40 Unstructured Grid*

*Figure 4 – Three Discretization Schemes on 80 x 80 Unstructured Grid*

The solution to *Eqn. 1* contains a discontinuity, so the survey line with the steepest slope is the most accurate. The survey lines become more accurate with increasing fineness of the meshes. The linear scheme only works on the structured grid because it is a central approximation and cannot solve on unstructured grids with arbitrary meshes. The linear upwind scheme is not very diffusive, as it produces a relatively steep slope, but it does produce new extrema on the ends of the discontinuity. The upwind scheme is first order accurate and relatively diffusive. Therefore, it does not produce a slope as steep as the linear upwind or van Leer schemes on any of the grids. The van Leer scheme is the least diffusive with the steepest slope on all of the grids, and it is higher order accurate. Also, it produces fewer new extrema and extrema closer to the real solution than the linear upwind scheme. However the van Leer scheme did require an Eulerian discretization of time to solve on the unstructured grids. As of now, the van Leer scheme is preferred due to its accuracy and creation of few new extrema.

**Question 2 – Limiter Comparison**

*Figure 5 – Four Gradient Limiters for Linear Upwind Scheme on 20 x 20 Unstructured Grid*

As stated previously, the linear upwind scheme produces new extrema along the survey lines. Therefore, it is an interesting candidate for the implementation of a limiter. *Figure 5* shows the linear upwind scheme used with four different limiters on a 20 x 20 unstructured grid. The faceMDLimiter limiter produces the steepest slope but is the worst at limiting the production of new extrema. The cellMDLimited and cellLimited limiters produce similar survey lines with slopes comparable to the faceMDLimiter limiter and less new extrema. The faceLimited limiter is the best at limiting the production of new extrema, but it is the worst at modeling the discontinuity.

**Question 3 – Uncertainty and Error**

An uncertainty analysis was performed in accordance with the ASME guidelines. The T values from the three unstructured meshes were compared. To try to get a sense of the overall uncertainty of the schemes, three points were chosen along the survey lines where the real solution contains the discontinuity.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Nx | Nz | ΔAi | Ni | hi |
| Mesh 3 – Coarse | 20 | 20 | 2.50E-03 | 400 | 0.0500 |
| Mesh 2 – Base | 40 | 40 | 6.25E-04 | 1600 | 0.0250 |
| Mesh 1 – Fine | 80 | 80 | 1.56E-04 | 6400 | 0.0125 |

*Table 1 – Summary of Meshes*

As seen, the ASME guideline of h1 < h2 < h3 was satisfied.

|  |  |  |
| --- | --- | --- |
|  | | ASME |
| N1, N2, N3 | 6400, 1600, 400 | N1 > N2 > N3 |
| r21 | 2.0 | r21 > 1.3 |
| r32 | 2.0 | r32 > 1.3 |

*Table 2 – Cell ratios and ASME Criteria*

Again, the necessary ASME criteria were satisfied. *Table 5* shows the observed order of accuracy and numerical uncertainty for the meshes at various y values.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Linear Upwind Scheme** | | | | |
|  | ASME Notation | y = 0.44 | y = 0.5 | y = 0.56 |
| T for Mesh 1 | ø1 | 1.0358 | 0.2600 | -0.0007 |
| T for Mesh 2 | ø2 | 0.9947 | 0.3581 | -0.0310 |
| T for Mesh 3 | ø3 | 0.8243 | 0.4021 | 0.0708 |
|  | ε32 | -0.1704 | 0.0440 | 0.1018 |
| ε21 | -0.0411 | 0.0981 | -0.0304 |
| s | 1.0000 | 1.0000 | -1.0000 |
| Order of Accuracy | p | 2.0503 | 1.1559 | 1.7453 |
|  | q(p) | 0.0000 | 0.0000 | 0.0000 |
| ø21ext | 1.0489 | 0.1802 | 0.0122 |
|  | ø32ext | 1.0489 | 0.3223 | -0.0743 |
| App. Rel. Error | e21a | 3.97% | 37.71% | 4,601.52% |
| App. Rel. Error | e32a | 17.13% | 12.29% | 328.13% |
| Extrap. Rel. Error | e21ext | 1.25% | 44.31% | 105.39% |
| Extrap. Rel. Error | e32ext | 5.17% | 11.12% | 58.24% |
| Numerical Uncertainty | GCI21fine | 1.58% | 38.38% | 2,444.86% |
| Numerical Uncertainty | GCI32coarse | 6.82% | 12.51% | 174.34% |

*Table 3 – Order of Accuracy and Numerical Uncertainty for the Linear Upwind Scheme*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Upwind Scheme** | | | | |
|  | ASME Notation | y = 0.44 | y = 0.5 | y = 0.56 |
| T for Mesh 1 | ø1 | 0.8651 | 0.3960 | 0.0596 |
| T for Mesh 2 | ø2 | 0.7854 | 0.4503 | 0.1173 |
| T for Mesh 3 | ø3 | 0.7120 | 0.4491 | 0.2127 |
|  | ε32 | -0.0734 | -0.0012 | 0.0954 |
| ε21 | -0.0797 | 0.0543 | 0.0576 |
| s | 1.0000 | -1.0000 | 1.0000 |
| Order of Accuracy | p | 0.1173 | 5.4576 | 0.7275 |
|  | q(p) | 0.0000 | 0.0000 | 0.0000 |
| ø21ext | 1.8054 | 0.3948 | -0.0282 |
|  | ø32ext | 1.6523 | 0.4503 | -0.0282 |
| App. Rel. Error | e21a | 9.21% | 13.70% | 96.61% |
| App. Rel. Error | e32a | 9.35% | 0.27% | 81.36% |
| Extrap. Rel. Error | e21ext | 52.08% | 0.32% | 311.27% |
| Extrap. Rel. Error | e32ext | 52.46% | 0.01% | 515.39% |
| Numerical Uncertainty | GCI21fine | 135.86% | 0.40% | 184.17% |
| Numerical Uncertainty | GCI32coarse | 137.95% | 0.01% | 155.09% |

*Table 4 – Order of Accuracy and Numerical Uncertainty for the Upwind Scheme*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **van Leer Scheme** | | | | |
|  | ASME Notation | y = 0.44 | y = 0.5 | y = 0.56 |
| T for Mesh 1 | ø1 | 0.9962 | 0.2871 | -0.0002 |
| T for Mesh 2 | ø2 | 0.9429 | 0.3703 | 0.0071 |
| T for Mesh 3 | ø3 | 0.7997 | 0.4076 | 0.1004 |
|  | ε32 | -0.1432 | 0.0373 | 0.0934 |
| ε21 | -0.0534 | 0.0832 | 0.0073 |
| s | 1.0000 | 1.0000 | 1.0000 |
| Order of Accuracy | p | 1.4236 | 1.1587 | 3.6835 |
|  | q(p) | 0.0000 | 0.0000 | 0.0000 |
| ø21ext | 1.0280 | 0.2196 | -0.0008 |
|  | ø32ext | 1.0280 | 0.3401 | -0.0008 |
| App. Rel. Error | e21a | 5.36% | 29.00% | 3,622.16% |
| App. Rel. Error | e32a | 15.19% | 10.07% | 1,321.27% |
| Extrap. Rel. Error | e21ext | 3.09% | 30.76% | 75.35% |
| Extrap. Rel. Error | e32ext | 8.28% | 8.90% | 968.12% |
| Numerical Uncertainty | GCI21fine | 3.98% | 29.41% | 382.15% |
| Numerical Uncertainty | GCI32coarse | 11.28% | 10.21% | 139.40% |

*Table 5 – Order of Accuracy and Numerical Uncertainty for the van Leer Scheme*

The scheme with the highest order of accuracy depends on which point is examined of the three. For y = 0.44, the linear upwind scheme has the highest order of accuracy; for y = 0.50, the upwind scheme has the highest; for y = 0.56, the van Leer scheme has the highest. The van Leer scheme has the second highest order of accuracy for y = 0.50 and y = 0.44, so one might say that this is the “most” accurate. However, the accuracy is dependent the selection of points. Therefore, the raw data were used to compute the order of accuracy using all possible points. The average orders of accuracy for the schemes were then determined. These appear below in *Table 6.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | | **Linear Upwind** | **Upwind** | **van Leer** |
| Average Order of Accuracy | pavg | 5.7000 | 5.8695 | 7.1697 |

*Table 6 – Average Orders of Accuracy for Three Discretization Schemes*

According to this methodology, the van Leer scheme has the highest order of accuracy. This is consistent with *Figures 2-4*, but an Eulerian discretization of time was needed in order to produce survey lines on the unstructured grids using the van Leer scheme.