Modelling atmospheric flows on 3D hybrid unstructured meshes using high-order methods

3rd EULAG Workshop

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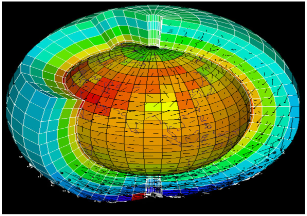
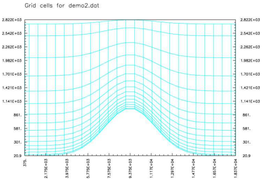
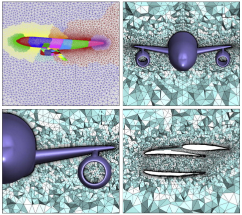
Unstructured Grids







Challenges

Challenges

- Inefficient representation of complicated orography
- Singularities at poles
- Formulation of governing equations
- Conservation of mass, and energy
- Efficient use of computanional resources
- Scalability at Teraflops and Petaflops HPC facilities

Initiatives

Initiatives by leading Research Centres

- UK Met Office and ECMWF (ENDGame)
- NCAR (High-Order Methods Modeling Environment)
- NOAA (AM3, NIM)
- DWD & Max Planck (ICON)

Selected Approach

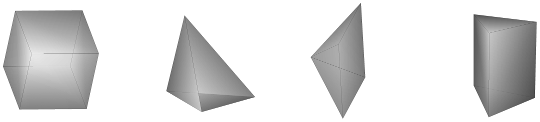
Outline

- Proposed framework is for first time applicable to arbitrary unstructured meshes and very high-order methods.
- Tsoutsanis et al., JCP & Comm. Comp. Phys.,2011
- High-order WENO up to 9th order accurate
- WENO HLLC Riemann solver
- Computer code UCNS3D; an extension of the in-house CNS3D (used for shock physics, turbulent mixing) to unstructured grids.

Element Shapes

Element Shapes

- Generated by mesh generation software packages
- Hexahedrals, tetrahedrals, pyramidal, prismatic elements
- Only conforming meshes considered
- Computational efficiency proportional to node count



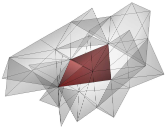
(a) Hexahedral (b) Tetrahedral (c) Pyramidal (d) Prismatic

Figure: Element Shapes

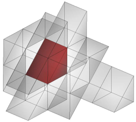
Central Stencil Selection

Procedure

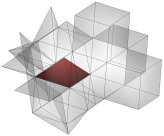
- For each element of the mesh
- Recursively add its direct side neighbours
- Exclude elements already in the stencil
- Stencils of various elements shapes are constructed



(a) Tetrahedral

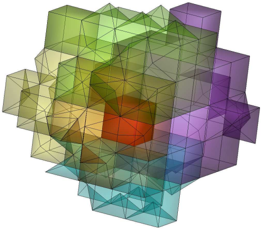


(b) Prismatic

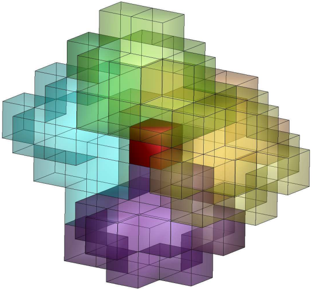


(c) Mixed

Directional Stencils



(a) Hybrid mesh



(b) Hexahedral mesh

Figure: Directional Stencils

Linear

Framework

- For each cell V_0 we would like to build a high-order polynomial $p(x, y, z)$ that has the same cell average as $u(scalar)$ on the target cell as well as averages $\bar{u}_m$ from the reconstruction stencil formed by neighbouring cells V_m
- $\overline{u}_0 = \frac{1}{V_0} \int\limits_{V_0} u(x, y, z)\, dV$
- Reconstruction carried out not in physical coordinates (x, y, z) but in a reference coordinate system (ξ, η, ζ)
    - Decompose each element into tetrahedrals and choose one of the decomposed tetrahedral elements
    - Transform the chosen element from physical to reference coordinates
    - Based on the Jacobian of the transformation, map the coordinates of the entire element into reference coordinates
    - Based on the same Jacobian recompute coordinates, barycentres, volumes of all the elements in the stencil in reference space

Linear

Framework

- The r^{th} order reconstruction polynomial at the transformed cell V_0' is sought as an expansion over local polynomial basis functions $\phi_k(\xi, \eta, \zeta)$
- $p(\xi, \eta, \zeta) = \sum_{k=0}^{K} a_k \phi_k(\xi, \eta, \zeta) = \bar{u}_0 + \sum_{k=1}^{K} a_k \phi_k(\xi, \eta, \zeta)$
- a_k are degrees of freedom and K is related to the order of the polynomial r, K=1/6(r+1)r+2)(r+3)
- The conservation condition must be satisfied
- For Hybrid meshes the basis function ϕ_k must be constructed in such a way that they satisfy the conservation condition
- $\phi_k(\xi, \eta, \zeta) \equiv \psi_k(\xi, \eta, \zeta) - \frac{1}{|V_0'|} \int_{V_0'} \psi_k \; d\xi d\eta d\zeta, \quad k = 1, 2, \ldots$ where

  $\{\psi_k\} = \xi, \;\; \eta, \;\; \zeta, \;\; \xi^2, \;\; \eta^2, \;\; \zeta^2, \;\; \xi \cdot \eta, \;\; \xi \cdot \zeta, \;\; \zeta \cdot \eta, \;\; \xi \cdot \eta \cdot \zeta \ldots$

Linear

Framework

- To find the unknown degrees of freedom a_k the conservation condition must be satisfied
- $\int_{E'_m} p(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = |V'_m|\bar{u}_0 + \sum_{k=1}^{K}\int_{V'_m} a_k\phi_k\, d\xi d\eta d\zeta = |V'_m|u_m, \quad m = 1,\ldots M$
- $A_{mk} = \int_{V'_m} \phi_k\, d\xi d\eta d\zeta, \quad b_m = |V'_m|(\bar{u}_m - \bar{u}_0)$
- $\sum_{k=1}^{K} A_{mk}a_k = b_m, \quad m = 1,2,\ldots M$
- least-square reconstruction of $\mathcal{F} = \sum_{m=1}^{M}\omega_m \cdot \left(\sum_{k=1}^{K} A_{mk}a_k - b_m\right)^2$ with ω_m being squared reciprocals of the distance
- QR decomposition employed for the least square solution

WENO

Framework

- High-order accurate and non-oscillatory behaviour
- Successfully applied and widely adopted in FV framework for structured and unstructured meshes (tetrahedrals in 3D by Tsoutsanis, Dumbser, Shu etc)
- The actual reconstructed value is a convex combination of reconstructed values from stencils, with nonlinear (solution-adaptive) WENO weights
- Nonlinear weights are constructed from the linear (constant) weights by taking into account smoothness of the solution in each of the reconstruction stencils
- Reconstruct entire polynomials
- First FV implementation of WENO for hybrid unstructured meshes in 3D retaining the characteristics of the scheme

WENO

Procedure

- The WENO reconstruction stencils is a union of several reconstruction stencils $\mathcal{S}_m, \; m = 0, 1, \ldots, m_s$
- WENO reconstruction polynomial $p_{\mathrm{weno}} = \sum_{m=0}^{m_s} \omega_m p_m(\xi, \eta, \zeta)$
- For each individual polynomial corresponding to the stencil $\mathcal{S}_m, p_m(\xi, \eta, \zeta) = \sum_{k=0}^{K} a_k^{(m)} \phi_k(\xi, \eta, \zeta)$
- $p_{\mathrm{weno}} = \bar{u}_0 + \sum_{k=1}^{K} \left(\sum_{m=0}^{m_s} \omega_m a_k^{(m)} \right) \phi_k(\xi, \eta, \zeta) \equiv \bar{u}_0 + \sum_{k=1}^{K} \tilde{a}_k \phi_k(\xi, \eta, \zeta)$
- the nonlinear weights are defined as $\omega_m = \frac{\gamma_m}{\sum_{m=0}^{m_s} \gamma_m}, \quad \gamma_m = \frac{d_m}{(\varepsilon + IS_m)^p}$
- d_m are the so-called linear weights, IS_m are smoothness indicators, ε is a small number used to avoid division by zero and finally p is an integer parameter
- The oscillation indicators IS_m of each stencil $IS_m = \sum_{1 < |\beta| < r} \int_{V_0'} \left(D^{\beta} p_m(\xi, \eta, \zeta) \right)^2 d\xi d\eta d\zeta$

Equations

- Three-dimensional Euler equations in the following formulation $\frac{\partial}{\partial t}\mathbf{U}+\frac{\partial}{\partial x}\mathbf{F}(\mathbf{U})+\frac{\partial}{\partial y}\mathbf{G}(\mathbf{U})+\frac{\partial}{\partial z}\mathbf{H}(\mathbf{U})=\mathbf{0}$
- Integrating in space over a mesh element V_i, and be exploiting the rotational invariance property of the Euler equations we obtain $\frac{d}{dt}\mathbf{U}_i+\frac{1}{|V_i|}\oint\limits_{\partial V_i}\mathbf{F}_n dA=$ $\mathbf{0}, \quad \mathbf{F}_n(\mathbf{U})=\mathbf{F}(\mathbf{U})\,n_x+\mathbf{G}(\mathbf{U})\,n_y+\mathbf{H}(\mathbf{U})\,n_z=\mathbf{T}^{-1}\mathbf{F}(\mathbf{T}\mathbf{U})$
- Numerical fluxes and initial solution approximated by a Gaussian quadrature of appropriate order
- The integral over the element boundary ∂V_i splits into the sum of integrals $\frac{d}{dt}\mathbf{U}_i=\mathbf{R}_i, \quad \mathbf{R}_i=-\frac{1}{|V_i|}\sum_{j=1}^{L}\int\limits_{A_j}\mathbf{F}_{n,j}dA=-\frac{1}{|V_i|}\sum_{j=1}^{L}\mathbf{K}_{ij}$
- The numerical flux given by $\mathbf{K}_{ij}=\int\limits_{A_j}\mathbf{F}_{n,j}dA=\sum_{\beta}\mathbf{F}_{n,j}\left(\mathbf{U}(\mathbf{x}_\beta,t)\right)\omega_\beta|A_j|$

Reconstruction

- WENO reconstruction is carried out in characteristic variables
- Polynomials given by $\mathbf{P}_{im}(\xi,\eta,\zeta) = \sum_{k=0}^{K} \mathbf{A}_{ik}^{(m)} \phi_{ik}(\xi,\eta,\zeta) = \bar{\mathbf{U}}_i + \sum_{k=1}^{K} \mathbf{A}_{ik}^{(m)} \phi_{ik}(\xi,\eta,\zeta),$
- Define as the arithmetic average of the conserved vector $\mathbf{U_i}$,$\mathbf{U}'_n = \frac{1}{2}(\mathbf{U}_i + \mathbf{U}_{i'})$
- Compute the matrices containing the right and left eigenvectors of the Jacobian matrix
- Compute the characteristic projections of vector degrees of freedom of each stencil S_m, including the cell averaged value $\mathbf{U_I}$ as $\mathbf{B}_{ikj}^{(m)} = \mathbf{L}_j \mathbf{A}_{ik}^{(m)}, \quad m = 0,\ldots,m_s, \quad k = 0,\ldots K.$
- The resulting modified degrees of freedom $\tilde{\mathbf{B}}_{ikj}^{(m)}$ are projected back to by multiplying them by $\mathbf{R_j}$
- The resulting WENO reconstruction polynomial for the face A_j is given by

$$\mathbf{P}_{ij}(\xi,\eta,\zeta) = \bar{\mathbf{U}}_i + \sum_{k=1}^{K} \tilde{\mathbf{A}}_{ikj} \phi_{ik}(\xi,\eta,\zeta), \quad \tilde{\mathbf{A}}_{ikj} = \mathbf{R}_j \mathbf{B}_{ikj}$$

Numerical Flux

Framework

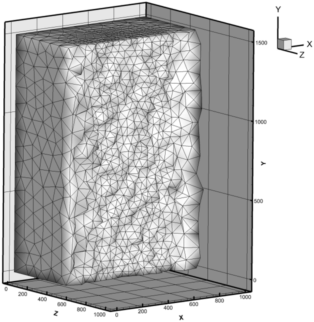
- Two approximate values for the conserved vector $\mathbf{U}$ at each Gaussian quadrature point exist
- The first value $\mathbf{U}_{\beta}^{-}$ corresponds to the spatial limit to the cell boundary from inside the cell V_i and the second value $\mathbf{U}_{\beta}^{+}$ corresponds to the spatial limit from outside the element
- HLLC Riemann solver employed
- Using the concept of the rotational invariance we rotate the data states $\mathbf{U}_{\beta}^{-}$,$\mathbf{U}_{\beta}^{+}$ in the direction of the normal flux vector , then employ the HLLC Riemann solver, and rotate back the numerical flux obtained from HLLC Riemann solver

Time Advancement

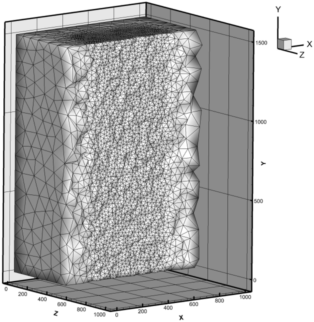
Time Advancement

- Scheme used is the explicit 3^{rd}-order TVD Runge-Kutta
- time step Δt is selected according to the formula $\Delta t = K \min_i \frac{h_i}{S_i \cdot V_i}$
- $K \leq 1/3$ is the CFL number
- the characteristic length h_i of each element is taken to be the radius of the inscribed sphere of each element
- For higher than 3rd-order schemes 3^{rd}-order TVD Runge-Kutta employed for convergence studies with time step size given by $\Delta t = K \cdot (\Delta x)^{\frac{n}{3}}$

Meshes Used



(a) Mesh1



(b) Mesh2

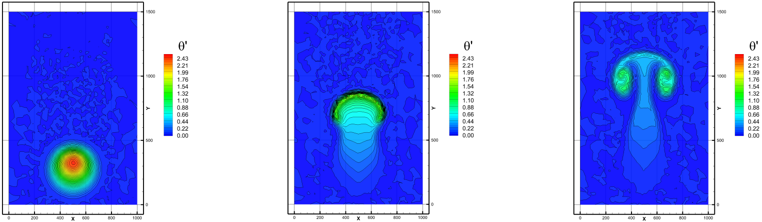
Figure: Meshes used

Problem Description

Description

- We solve $\frac{\partial}{\partial t}\mathbf{U} + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{U}) + \frac{\partial}{\partial y}\mathbf{G}(\mathbf{U}) + \frac{\partial}{\partial z}\mathbf{H}(\mathbf{U}) = \mathbf{S}$
- Warm bubble centered at $(500, 260, 500)\ m$
- $\theta' = \begin{cases} 0 & \textit{for}\ r > r_c \\ 1.25\left(1 + cos\left(\frac{\pi r}{r_c}\right)\right) & \textit{for}\ r \geq r_c \end{cases}$
- The computational domain is $[0, 1000]\,x\,[0, 1500]\,x\,[0, 1000]\ m$.
- NFBC used at the boundaries
- Simulation time $t \in [0, 300]\ s$

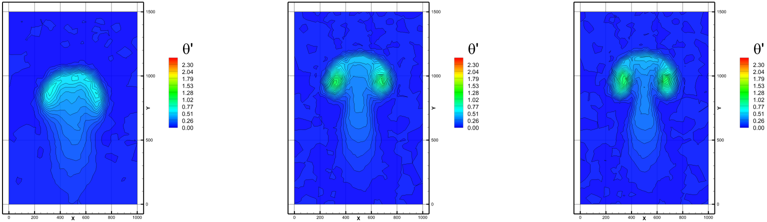
Results



(a) $t = 50sec$ (b) $t = 200sec$ (c) $t = 300sec$

Figure: Potential temperature perturbation θ'at various instants and at $z = 500m$ for mesh2 using WENO-5th order scheme.

Results



(a) TVD-2nd (b) WENO-3rd (c) WENO-5th

Figure: Potential temperature perturbation θ'at $t = 300sec$ and at $z = 500m$ for mesh1.

Results

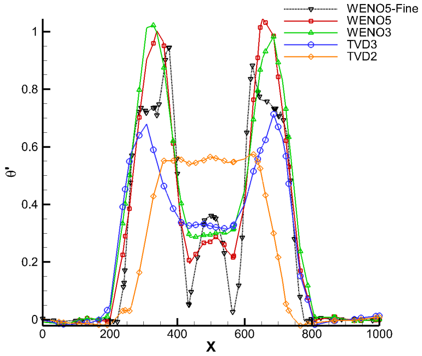
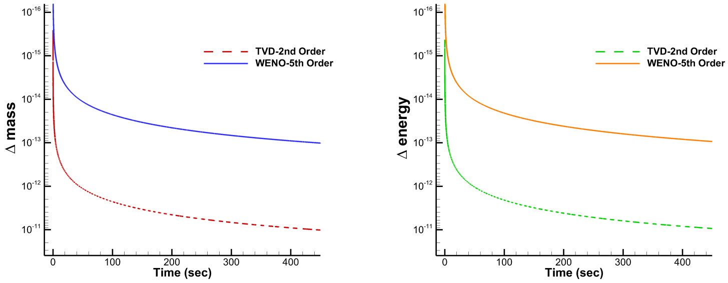


Figure: Potential temperature perturbation θ'(K) at $t = 300sec$ profile, at $z = 500m$ and $y = 964.5m$.

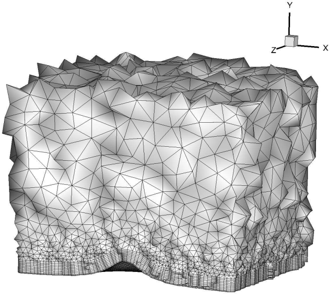
Conservation properties



(a) Mass (b) Energy

Figure: Conservation properties of different schemes

Meshes Used



(a) Mesh1 (b) Mesh3

Figure: Meshes used

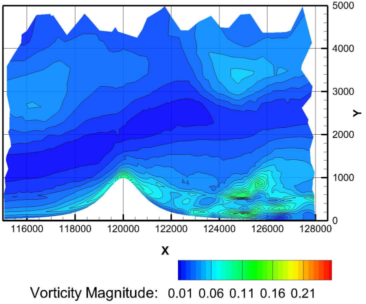
Problem Description

Description

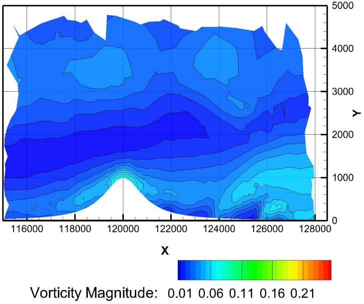
- We solve $\frac{\partial}{\partial t}\mathbf{U} + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{U}) + \frac{\partial}{\partial y}\mathbf{G}(\mathbf{U}) + \frac{\partial}{\partial z}\mathbf{H}(\mathbf{U}) = \mathbf{S}$
- Defined on $[110, 130] \times [0, 12] \times [110, 130]km$ with NFBC on the ground and NRBC elsewere
- The initial condition corresponds to a constant mean flow of $\bar{u} = 20m/s$ in a uniform stratified atmosphere and a ground temperature of $T_0 = 280K$
- Mountain profile given by $h(x, y, z) = \frac{h_c}{\left(1+\left(\frac{x-x_c}{a_c}\right)^2+\left(\frac{y}{a_c}\right)^2+\left(\frac{z-z_c}{a_c}\right)^2\right)}$

  with$h_c = 1000m$
- We compute the numerical solution at the output time $t = 1800sec$

Results



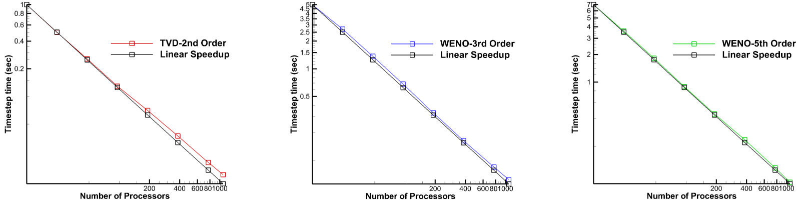
(a) Hybrid (Prisms, Tetrahedrals)



(b) Unstructured Tetrahedral

Figure: Vorticity magnitude at $t = 1800sec$ and $z = 120km$.

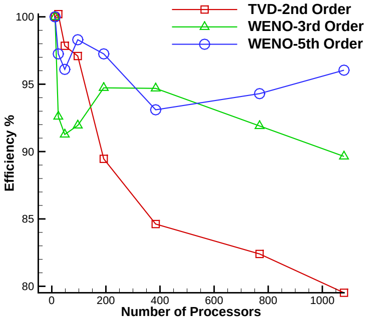
Parallel scalability



(a) TVD-2nd (b) WENO-3rd (c) WENO-5th

Figure: Scalability of various methods

Parallel efficiency



(a) Efficiency

Figure: Parallel efficiency of various methods

Conclusions

- The subcell resolution through decomposition and Gaussian quadrature integration rules is the mechanism that provides higher-accuracy on under-resolved meshes
- The crucial process for achieving high-order of accuracy is a reconstruction process that can combine elements of different shapes
- The subject schemes have been applied to a series of idealized test cases in order to assess their robustness, accuracy, and efficiency
- The numerical result obtained from the test cases demonstrated the aforementioned properties of the schemes
- The WENO reconstruction can be utilised as a building-block in a dynamical core that is not limited by the type of meshes, or the formulation of the governing equations.
- The higher-order schemes exhibit excellent scalability since the ratio of computational time over communication time is greater than lower order schemes
- In the future the extension of the current numerical methods to global idealized simutations will be implemented.

Questions?

Thank you very much for your time and attention !