CHARACTERISTICS-BASED FLUX-FORM SEMI-LAGRANGIAN METHODS FOR ATMOSPHERIC SIMULATION

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Outline

- Introduction
- Methods & Model
  - Characteristics-Based Flux-Form Semi-Lagrangian
  - Split-Explicit Time Stepping
- Future Work
  - Multi-Moment CB-FFSL
  - Genuinely Multi-Dimensional CB-FFSL

Scaling, Efficiency, & Effectiveness

- Modern architectures: 100,000+ processing cores
  - Models must scale massively parallel machines
  - Pass as few messages as possible
- Scaling + … = Efficiency
  - Time step
  - Single-node efficiency
- Efficiency + … = An Effective Model
  - Conservation
  - Oscillations & Positivity
  - Damping & Effective resolution
  - Isotropy & Grid imprinting
  - Properly balancing source terms and fluxes
    - Geostrophic, Hydrostatic, Thermal wind

The Extremes of Efficiency

- Semi-implicit semi-Lagrangian
  - Large time step
  - High single-node efficiency
  - Poor Scaling to 100,000+ processors
- Explicit Eulerian Galerkin Method
  - Small time step
  - Low single-node efficiency
  - Good scaling to 100,000+ processors
- Explicit CB-FFSL Finite-Volume Method
  - In between time step
  - In between single-node efficiency
  - Good scaling to 100,000+ processors

Explicit Integrators, Scalability, & Time Step

- Multi-Stage (e.g. Runge-Kutta)
  – Requires halo swap for each stage (more communication)
- Multi-Step (e.g. Adams-Bashforth)
  – Only one halo swap per time step (less communication)
  – CFL Limited to order unity
- Single-Stage Single-Step (i.e. Fully Discrete)
  – Only one halo swap per time step (less communication)
  – CFL larger than unity
  – Often used in atmospheric transport
  – Examples in transport
    - Lin-Rood FFSL
    - Conservative Semi-Lagrangian (CCS, SLICE, GeCORE, CSLAM)
    - ADER (Arbitrary accuracy DErivative Riemann) method

Explicit Semi-Lagrangian: From Transport to Non-Linear Equations

- Method of Characteristics
  - Transforms non-linear equation set into transport equations
  - Characteristic variables materially conserved along characteristic trajectories
  - Equation set must be hyperbolic
- Semi-Lagrangian Transport of Characteristics
  - FFSL method guarantees conservation & allows flexibility

Dry Atmospheric Euler Equations

- Dry, compressible, inviscid, & non-hydrostatic equations

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho u \\ \rho w \\ \rho\theta\end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix}\rho u \\ \rho u^2 + p \\ \rho uw \\ \rho u\theta\end{bmatrix} + \frac{\partial}{\partial z}\begin{bmatrix}\rho w \\ \rho wu \\ \rho w^2 + p \\ \rho w\theta\end{bmatrix} = \begin{bmatrix}0 \\ 0 \\ -\rho g \\ 0\end{bmatrix}$$

- Conserves:
  - Mass
  - Momentum
  - Potential Temperature (& therefore entropy)

L. A. Bauer, 1908, Phys. Rev.

$$s = c_p \log\theta + const$$

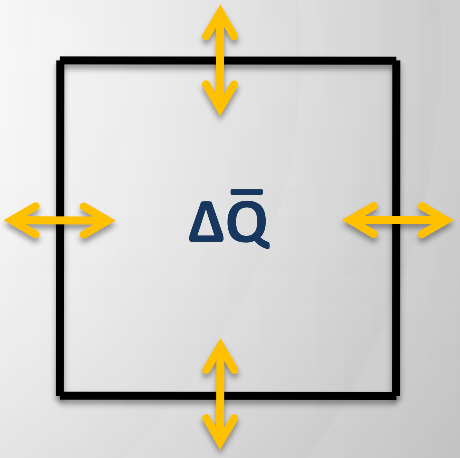
- Gravity source term
- Equation set is hyperbolic; thus allows characteristics

EXPLICIT EULERIAN FINITE-VOLUME

- Change in mean Q depends on flux through boundaries
- Fully Discrete: Time discretized by a direct integral
- We want to know the time-averaged flux through each cell boundary

$$\frac{\partial Q}{\partial t} + \frac{\partial F(Q)}{\partial x} + \frac{\partial H(Q)}{\partial z} = 0$$

$$\frac{\partial \overline{Q}}{\partial t} + \frac{1}{V_\Omega} \int_{\partial\Omega} \vec{F}(Q) \cdot \hat{n} \, d\Gamma = 0$$

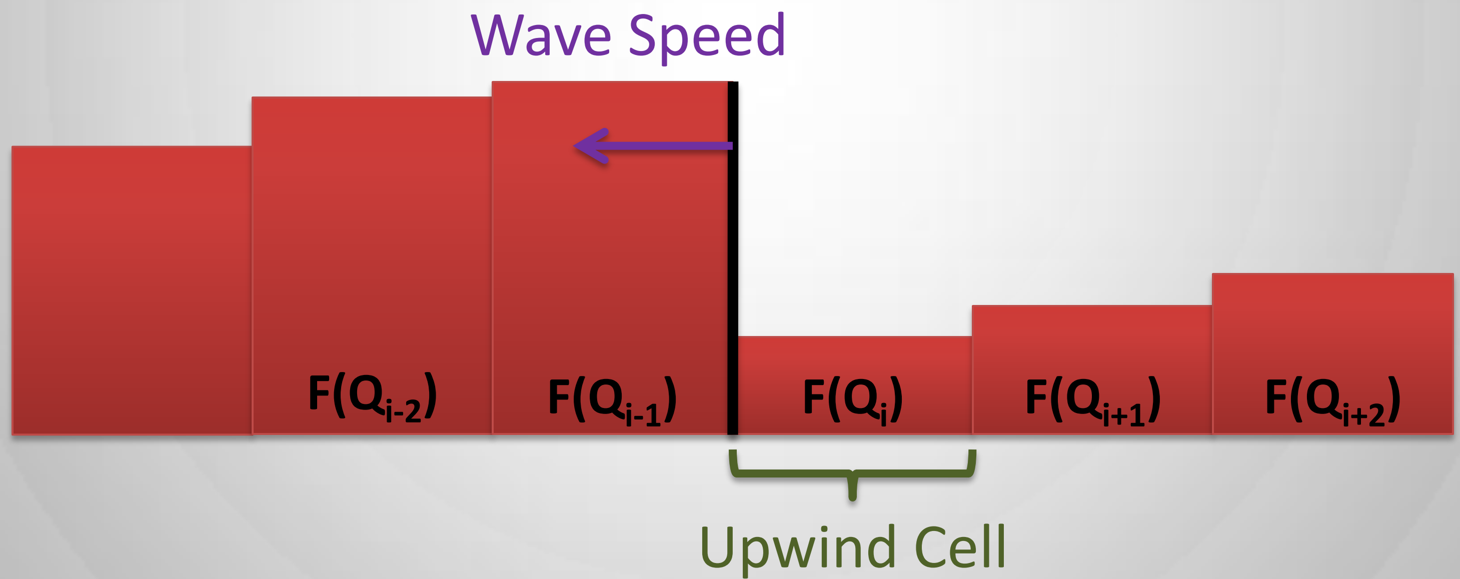


$$\overline{Q}^{\,n+1} = \overline{Q}^{\,n} - \frac{\Delta t}{V_\Omega} \sum_i \Gamma_i F^{\perp}_{avg,i}$$

Characteristics-Based FFSL Method

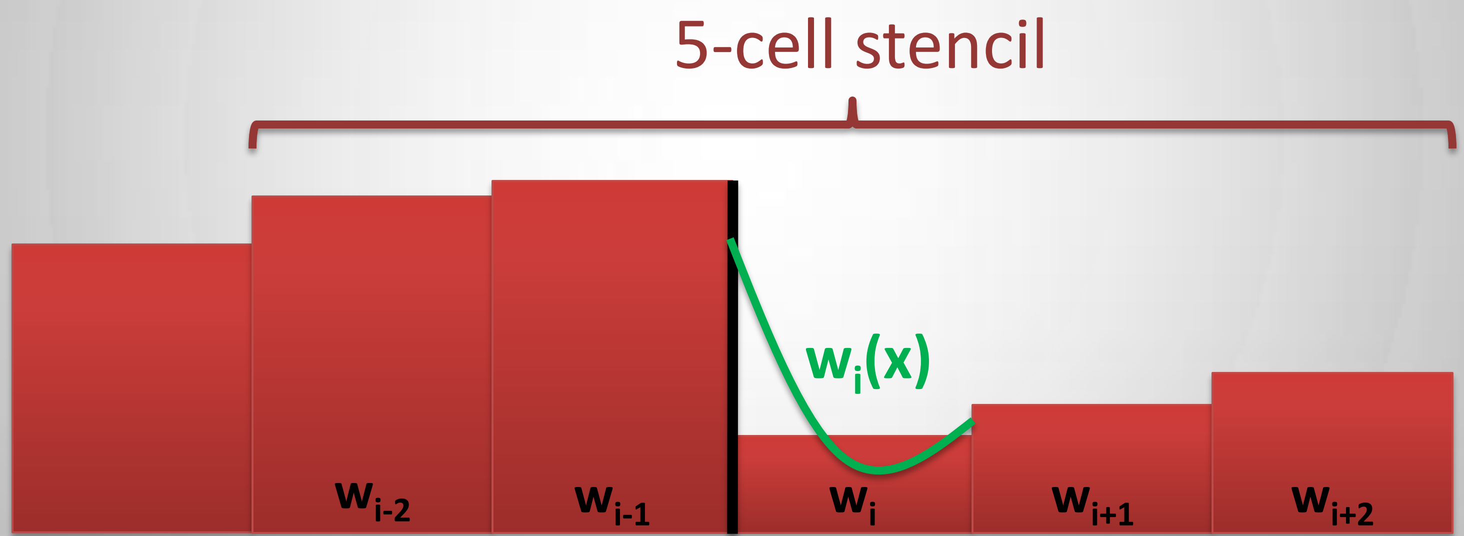
What is the flux at the cell boundary?

Decompose into characteristics



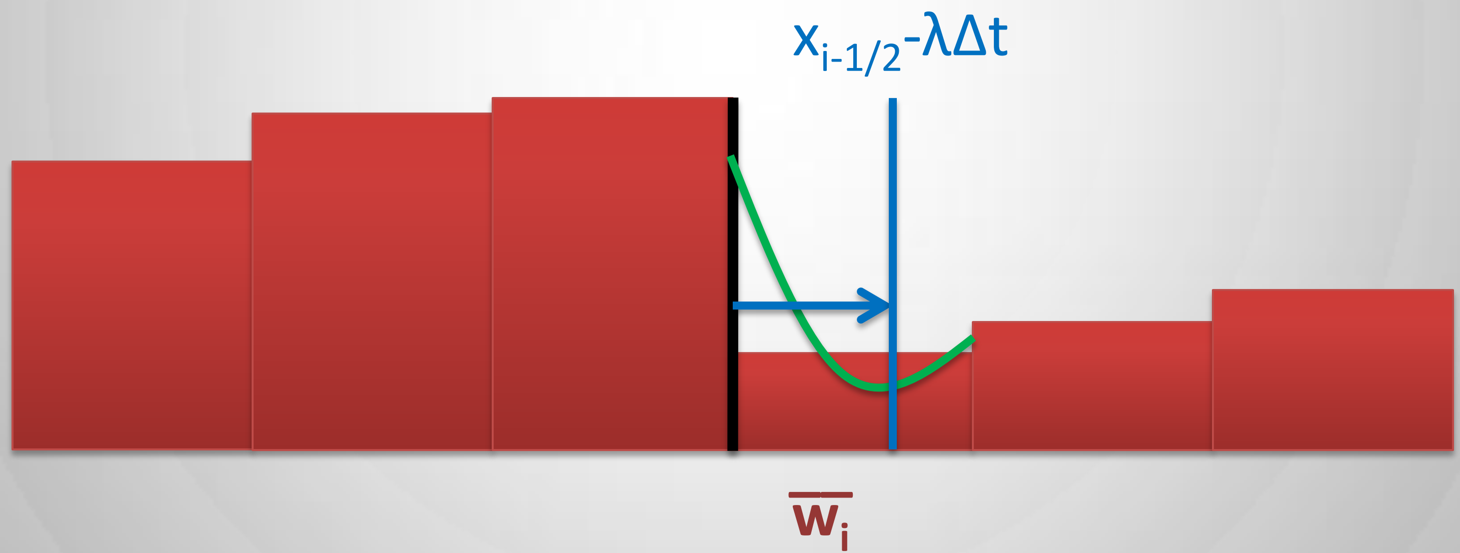
Characteristics-Based FFSL Method

Reconstruct Characteristic Var. for Upwind Cell



Characteristics-Based FFSL Method

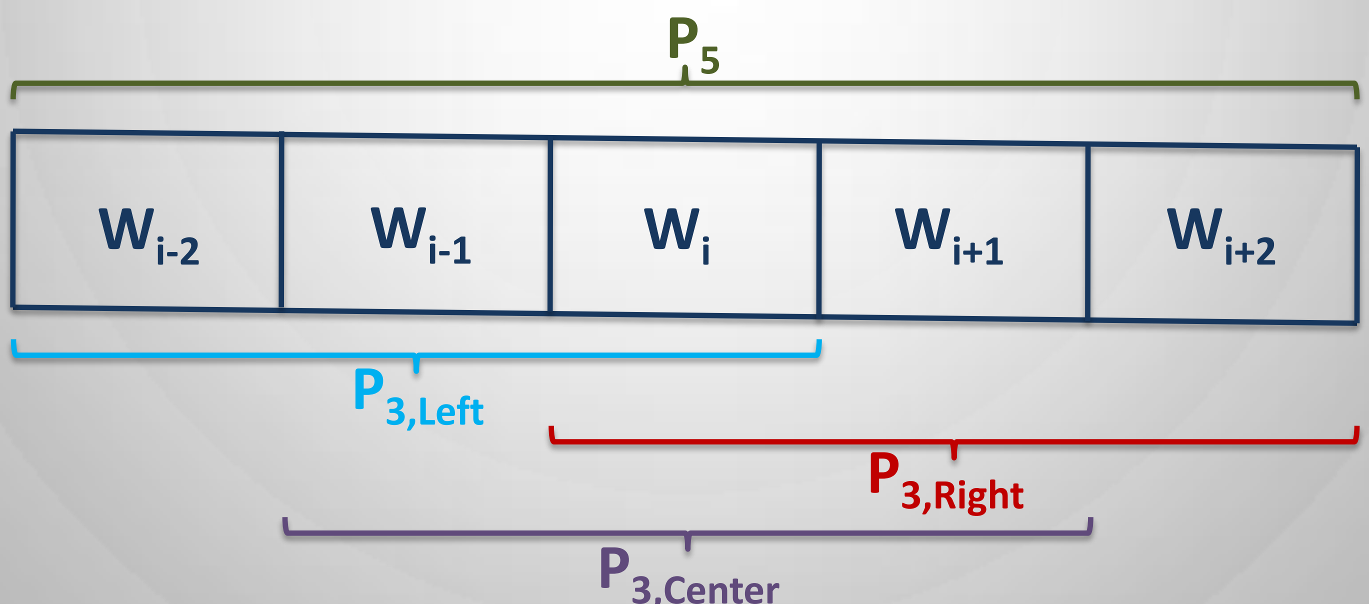
Time integral cast into upstream spatial integral over domain of dependence



Integrate w(x) over Domain of Dependence

Weighted Essentially Non-Oscillatory (WENO) Reconstruction (Shu 1999)

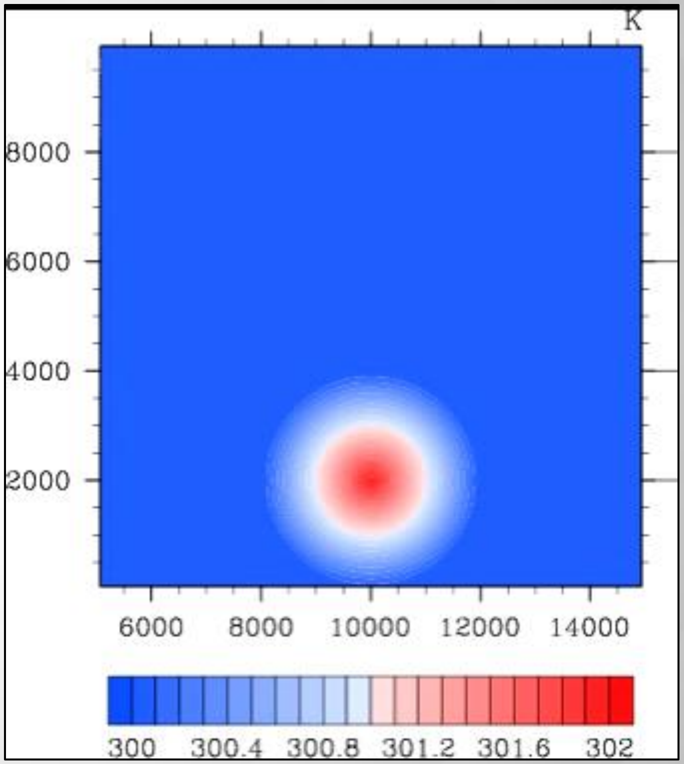
- Adaptive use of stencils
  - Create interpolants over multiple stencils
  - Compute the oscillations of each interpolant
  - Weight the most oscillatory interpolant the lowest
  - Use the weighted sum of the interpolants
  - Accuracy between 3rd and 5th order in the case below



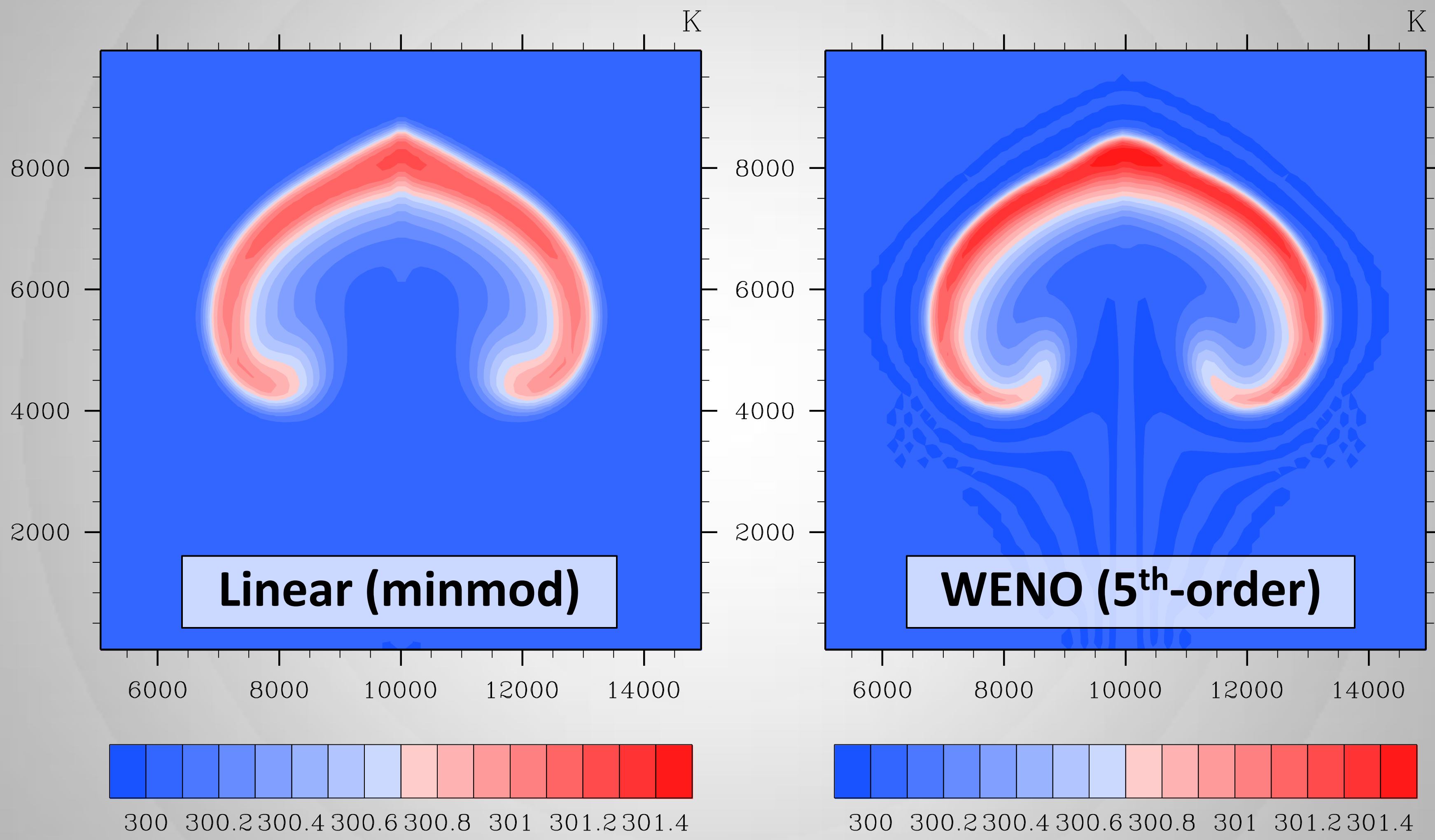
Convective Bubble Test Case

- Initial Conditions
  - Constant potential temperature
  - Hydrostatic balance
  - No wind
  - 2 °K potential temperature perturbation
- Simulated for 1,000 s
- $\Delta x = \Delta z = 150$ m
- CFL=0.9 ($\Delta t \approx 0.38$ s)

Wicker & Skamarock (1998, MWR)

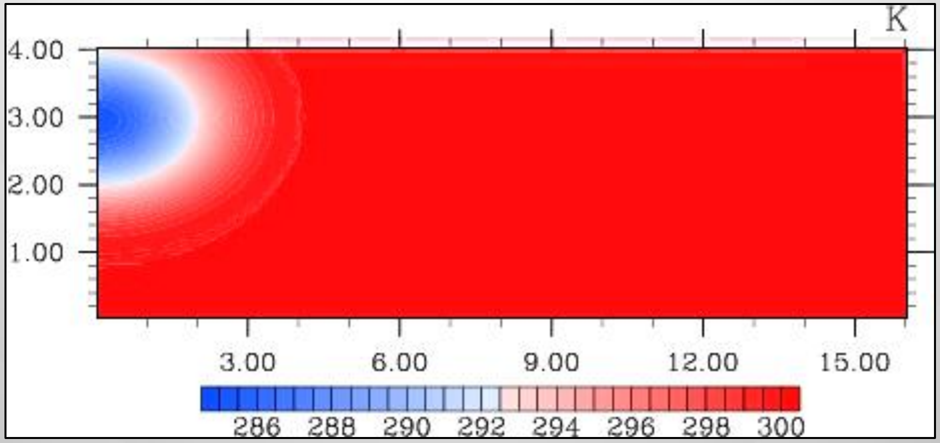


Convective Bubble Test Case

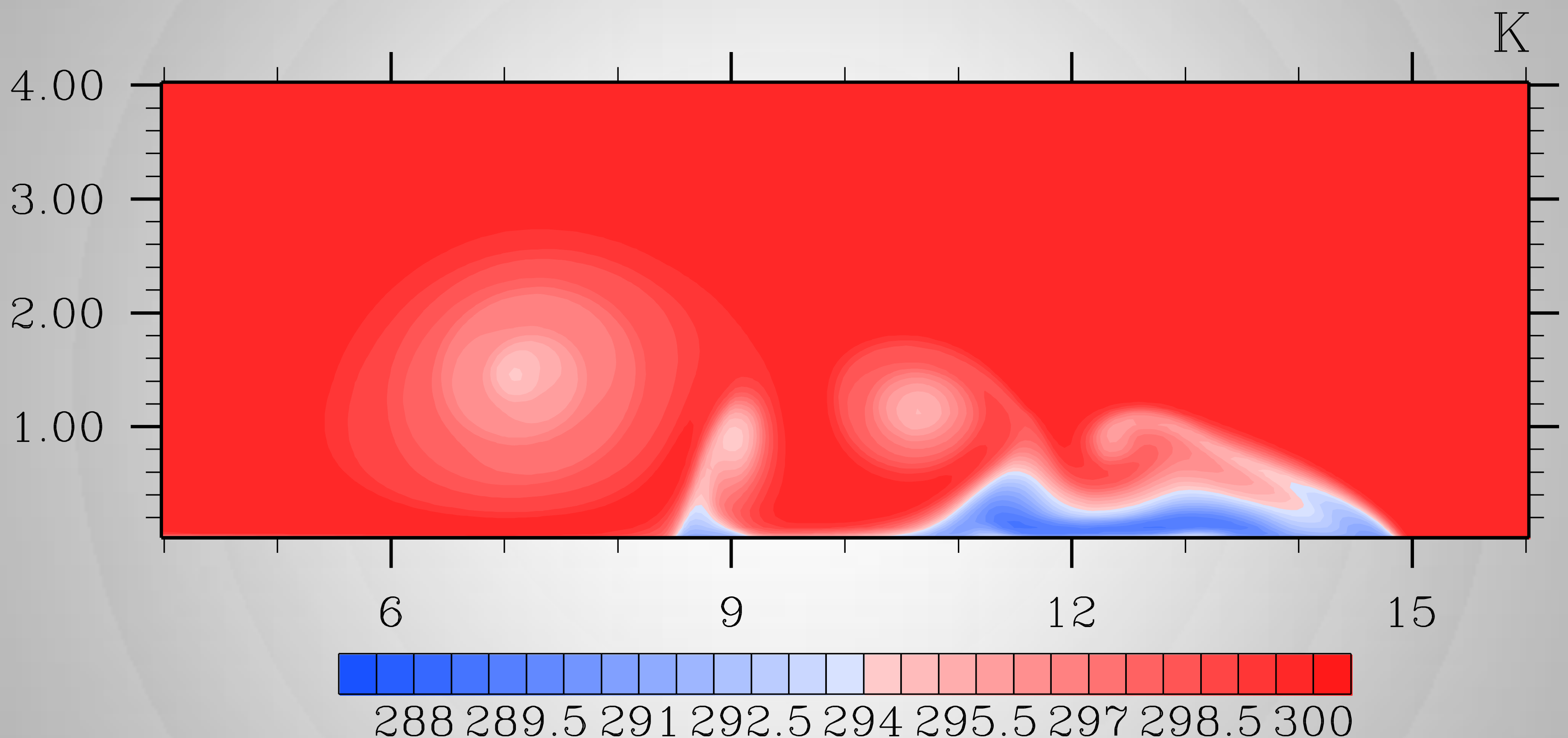


Straka Density Current Test Case

- Initial Conditions (Straka et al, IJNMF, 1993)
  - Constant potential temperature
  - hydrostatic balance
  - no wind
  - -15 °K potential temperature perturbation
- Simulated for 900 s
- $\Delta x = \Delta z = 50$ m
- CFL=0.9 ($\Delta t \approx 0.13$ s)

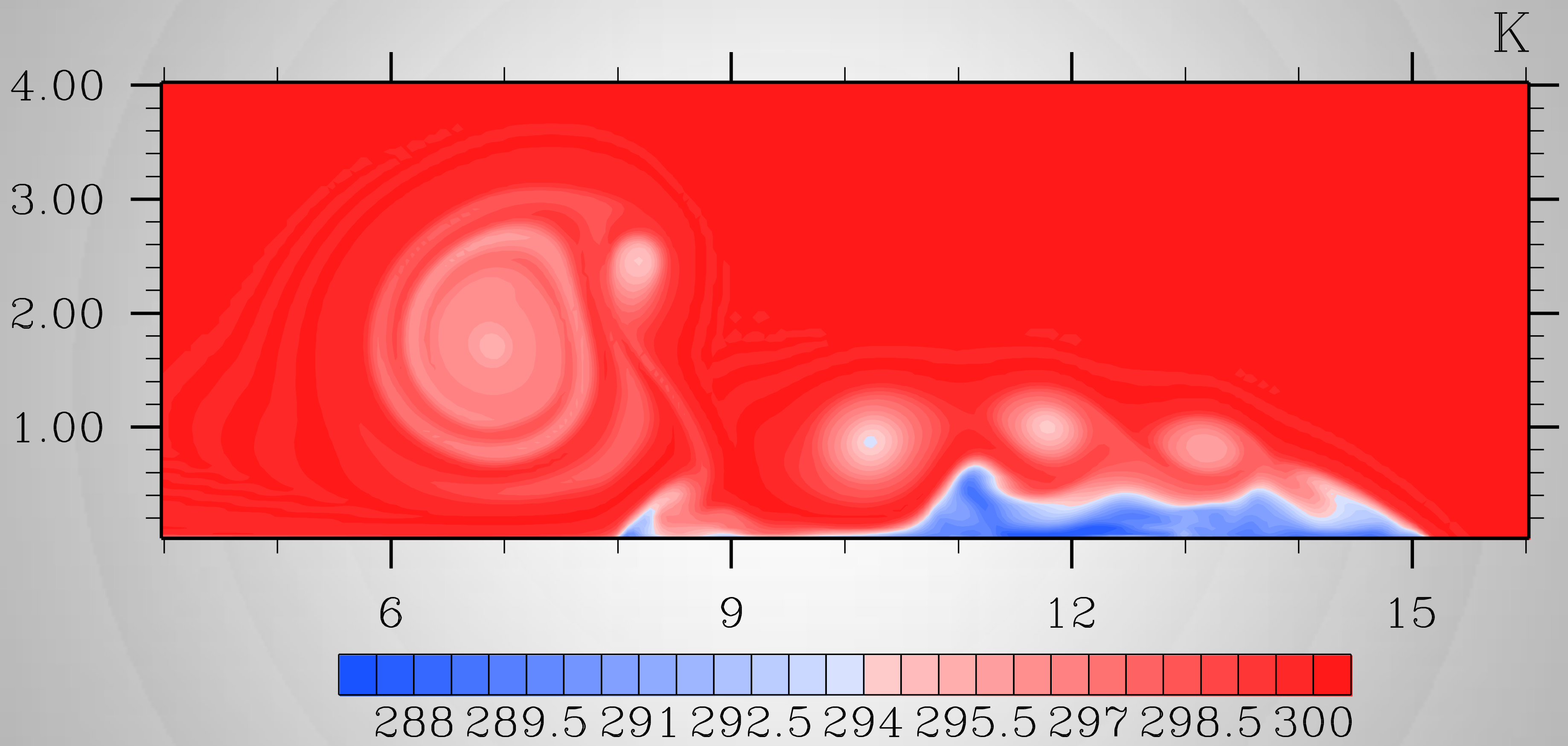


Straka Density Current Test Case: Results



Linear (minmod)

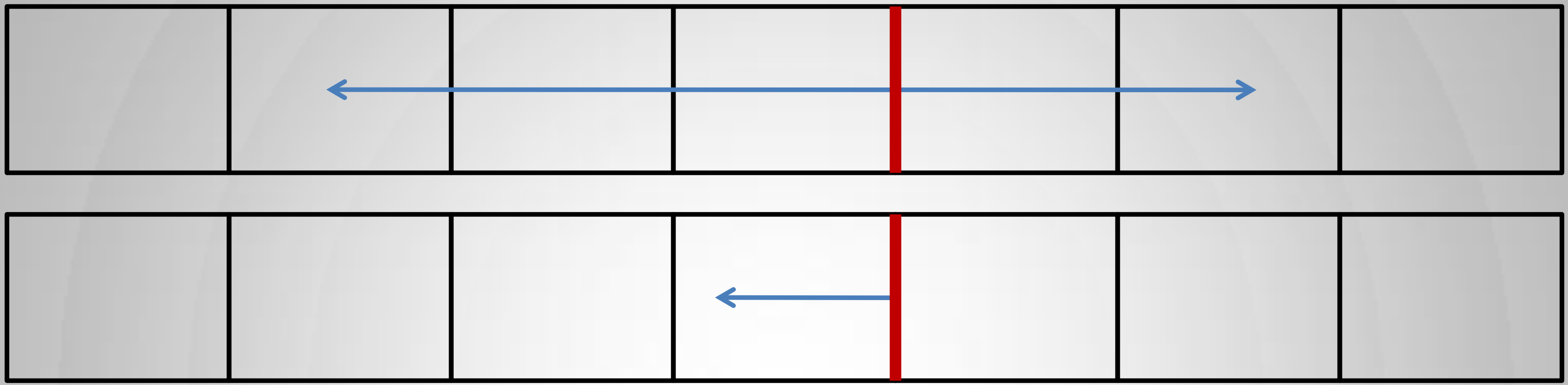
STRAKA DENSITY CURRENT TEST CASE: RESULTS



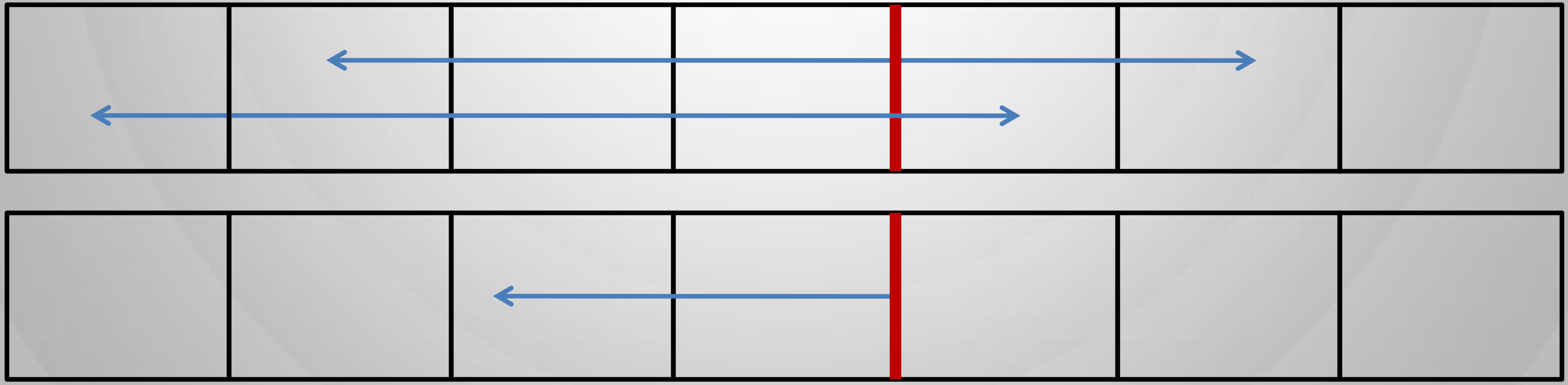
WENO (5th-order)

CFL > 1: An Example

- (CFL ≤ 1) + (5^{th}-order) = 3 halo transfers



- (CFL ≤ 2) + (5^{th}-order) = 4 halo transfers

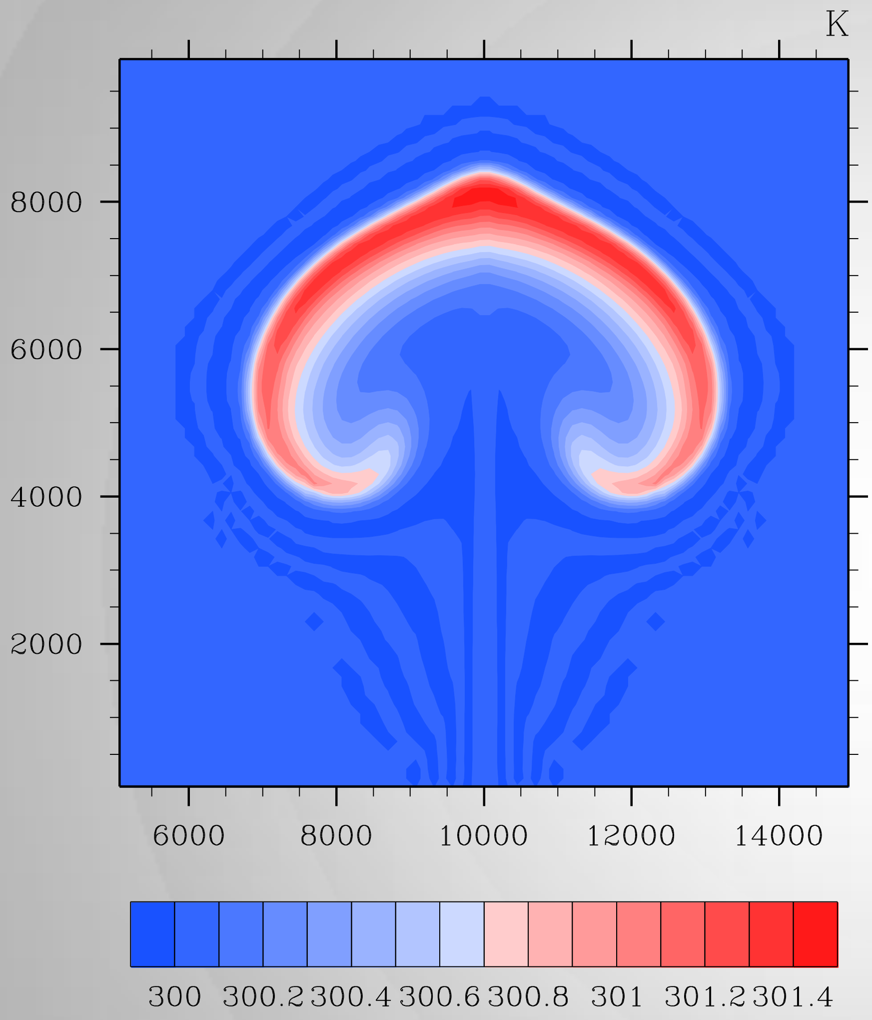


Split-Explicit Time Stepping

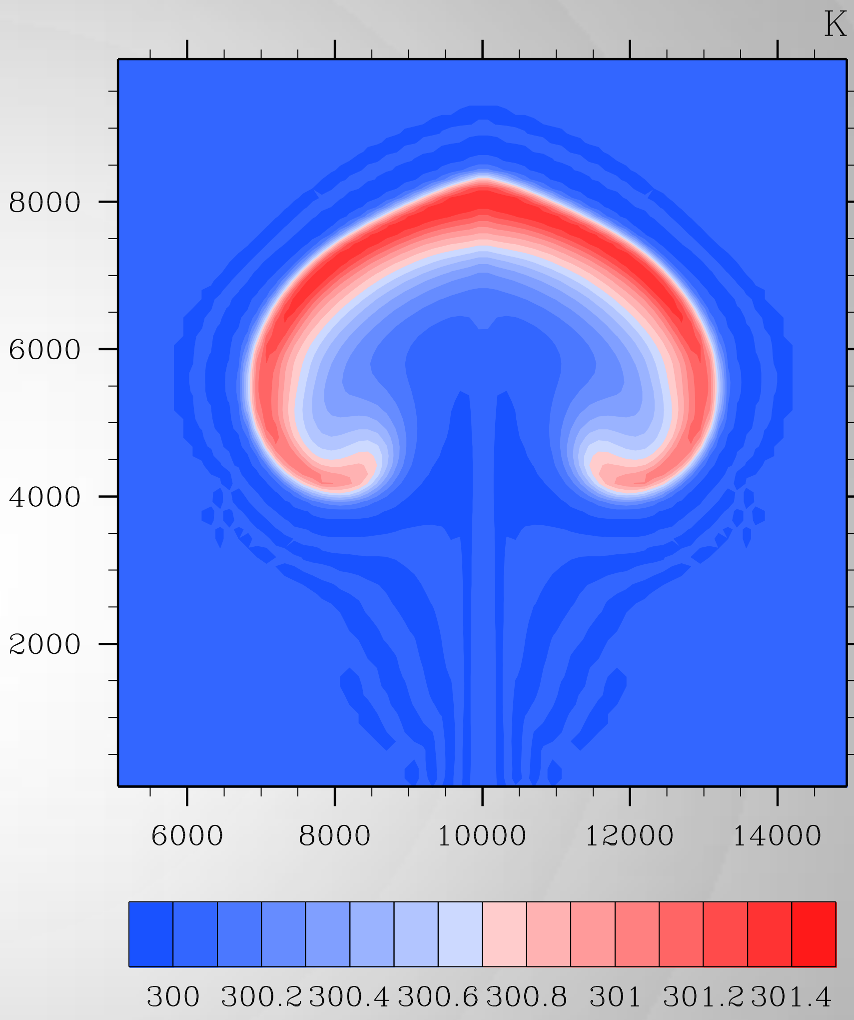
- Subcycle fast (acoustic) waves on a smaller time step
- Simulate slow (advection) waves on a larger time step
- 1st-order splitting error in equations
- Very easy to implement with characteristics
  - $\boxed{u, \quad u,}$ $\boxed{u+c_s, \quad u-c_s}$

    Slow Fast
- Implemented for rising thermal test case
  - 3 fast time steps per slow time step
  - WENO5 for slow waves & WENO5 for fast waves: 38% less CPU
  - WENO5 for slow waves & WENO3 for fast waves: 59% less CPU

Split-Explicit Time Stepping



WENO5 for slow, WENO5 for fast

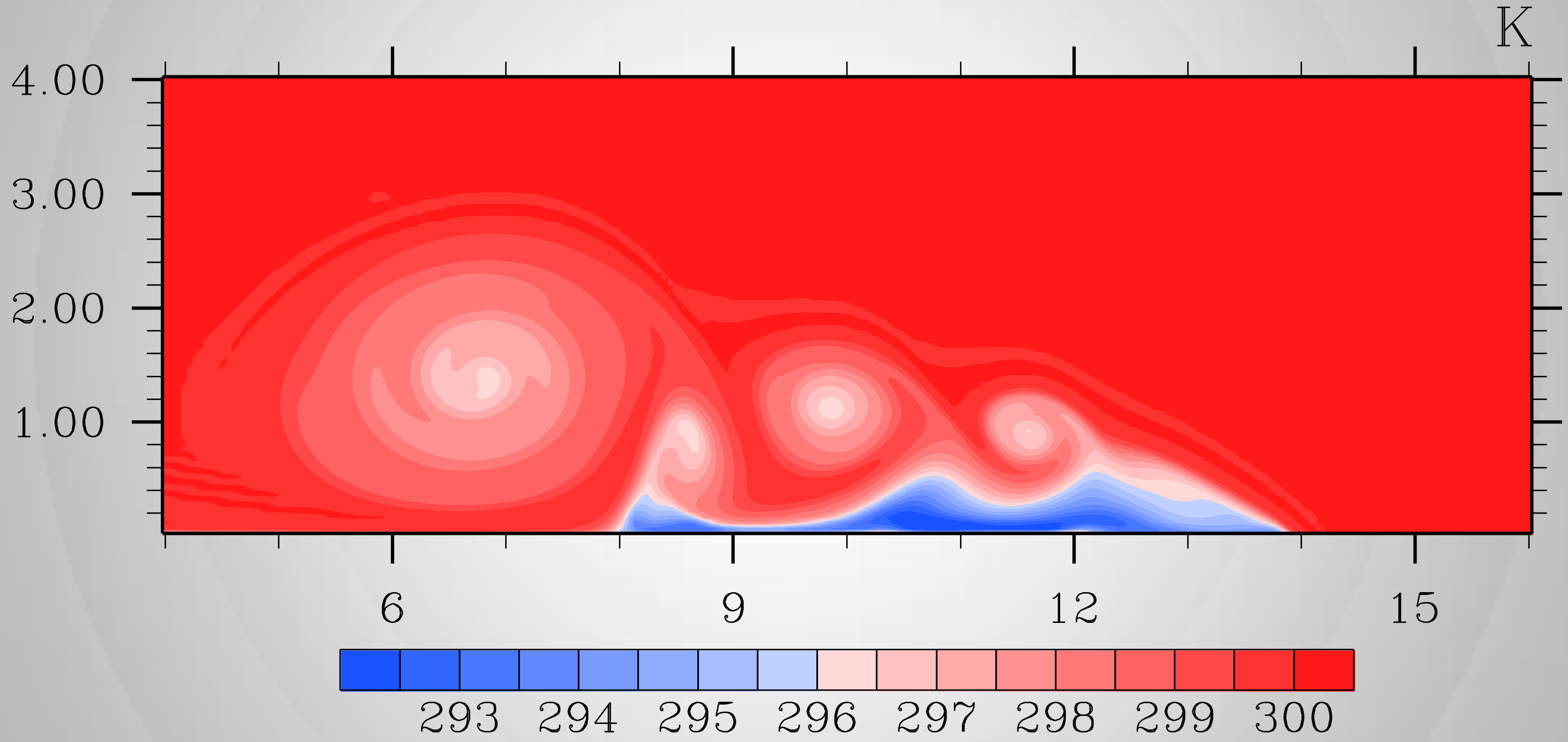


WENO5 for slow, WENO3 for fast

Is it worth it to use a cheaper method for fast waves?

Split-Explicit Time Stepping

10 fast time steps per slow time step: CFL=9.9



Multi-Moment Finite-Volume Method

- Evolve cell mean values & cell mean derivatives
- Reconstruction is more compact (fewer halo transfers)
- Assuming Jacobian is constant in time and uniform in space
  - Derivatives follow the same characteristics as values
- Value + 1st-derivatives: 3-cell stencil gives 6th-order accuracy
- Value + 1st + 2nd-derivatives: 3-cell stencil gives 9th-order accuracy
- Multi-moment is generally more accurate than single-moment for same order of accuracy
  - Evidenced by Prather scheme results (Prather, 1984, JGR)
  - Likely due to reconstruction stencil width
  - Coefficient Matters: $O[\Delta x^2]$ will probably be better than $O[(2\Delta x)^2]$

Multi-Moment Finite-Volume Method

- However, not certain how to couple with physics & boundaries
  - Physics alters cell means but not cell derivatives
  - Other coupled models (sea ice, land, ocean, etc.) may not alter derivatives
  - Derivatives then decouple from cell means and are no longer valid
  - To use invalid derivatives would act against the physics alterations
  - Probably leading to odd and unpredictable behavior!

<u>Seemingly only two options</u>

1. Reconstruct derivatives from altered cell means
   - Actually, this is <u>less</u> scalable than traditional FV
   - Likely forfeits the accuracy gain of going multi-moment as well
2. Derive physics parameterizations that evolve derivatives
   - Not an easy task, but possible
   - Requires coupled models to do the same

Genuinely Multi-Dimensional: Bicharacteristics

- Accounts for multi-dimensional nature of characteristics
  - Relaxes dependence on a rectangular mesh
  - Great isotropy on any mesh
  - Better tracer consistency with multi-dimensional transport
  - Greatly reduces error at cubed-sphere panel edges and corners
- Implementation is the key
  - Acoustic waves propagate along Mach cones
  - Various levels of approximation possible
  - Experimentation required to test approximations
- Possible application to characteristics-based DG methods

Linearized Acoustic Wave: Mach Cone

Trace acoustic wave back in time from point P

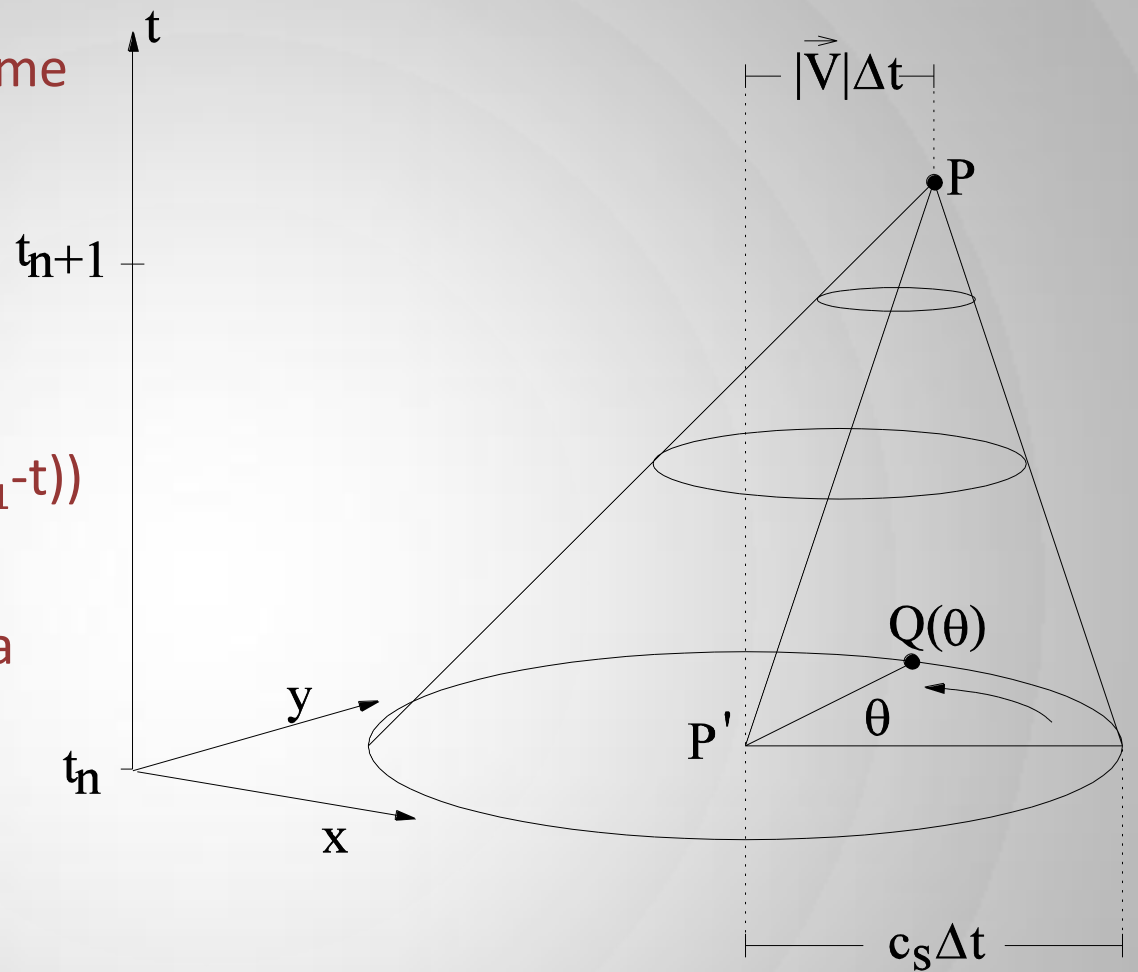
Renders a slanted cone

Radius: $c_s(t_{n+1}-t)$

Center: $(x-V_x(t_{n+1}-t)\ ,\ y-V_y(t_{n+1}-t))$

Computing state variables at a point in time and space from upstream values requires integration in time!

Advection waves are integrated as zero-radius Mach cones (solution is decoupled from θ)



BICHARACTERISTICS: PRACTICAL ISSUES

- Is it really worth it?
- Perhaps Not
  - Acoustic waves are not the dominant dynamical influence
  - It's not cheap
- Perhaps So
  - Splitting error is particularly large on the cubed-sphere
  - Maybe the best way to achieve multi-dimensional consistency with tracers
  - We could increase the sophistication of the advection wave integration
  - Only way to have no splitting & large CFL in an explicit method
- Only experimentation will decide
  - Likely depends on the CFL used

Thanks for Your Attention

Questions and Comments

High-Order & Hermite Reconstruction

- Many ways to reconstruct (e.g. 4^{th}-order)
  - Use 4 4^{th}-order accurate 0^{th}-order derivatives (Trad. FV)
  - Use 2 3^{rd}-order accurate 1^{st}-order derivatives
    & 2 4^{th}-order accurate 0^{th}-order derivatives (Mult. Mom. FV)
- Evolve multiple derivs. & use for compact reconstruction
- Most obvious in DG with Taylor basis
- Also done in nodal methods

CUBED-SPHERE GEOMETRY

- Why cubed-sphere?
  - Logically rectangular: Easy to reconstruct to arbitrary orders
  - Equiangular Gnomonic: computational grid of uniform squares
  - Near uniform cell area globally
  - Dimensional splitting trivial
- Difficulties when a stencil is required (e.g. FV, DG + HWENO)
  - Panel edges & corners: coord. system changes, cell geometry changes
  - High-order requires remapping onto extended local panel grid
  - Requires a halo exchange
  - Changing Jacobian reduces accuracy of reconstructions

Another Option for Sphere

- Local stereographic projection
  - Might as well go with a geodesic grid (triangles)
    - Isotropy is not sacrificed if bicharacteristics are used
  - Removes Jacobian gradient from the picture
  - Removes the need for a halo swap at panel edges / corners
  - Significantly complicates arbitrarily high-order 2-D reconstruction
    - May pre-compute Vandermonde-type matrix inversions (if non-singular!)
    - Likely not practical for evolving mesh

Characteristics

- Homogeneous Fluid Equations $$\frac{\partial Q}{\partial t} + \frac{\partial F(Q)}{\partial x} = 0$$
- Apply chain rule to flux $$\frac{\partial Q}{\partial t} + \boxed{\frac{\partial F}{\partial Q}}\frac{\partial Q}{\partial x} = 0$$

Flux Jacobian

- Diagonalize flux Jacobian into Eigenvectors and Eigenvalues

$$\frac{\partial F}{\partial Q} = R\Lambda R^{-1} \rightarrow \frac{\partial Q}{\partial t} + R\Lambda R^{-1}\frac{\partial Q}{\partial x} = 0$$

- Multiply equation by R^{-1} $$R^{-1}\frac{\partial Q}{\partial t} + \Lambda R^{-1}\frac{\partial Q}{\partial x} = 0$$
- Assume R^{-1} is constant & uniform $$\frac{\partial \left(R^{-1}Q\right)}{\partial t} + \Lambda\frac{\partial \left(R^{-1}Q\right)}{\partial x} = 0$$

CHARACTERISTICS

- Decoupled set of simple transport equations

$$\frac{\partial w_1}{\partial t} + \lambda_1 \frac{\partial w_1}{\partial x} = 0$$
$$\frac{\partial w_2}{\partial t} + \lambda_2 \frac{\partial w_2}{\partial x} = 0$$
$$\frac{\partial w_3}{\partial t} + \lambda_3 \frac{\partial w_3}{\partial x} = 0$$

$$W = R^{-1}Q = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$

- After transporting, retrieve state variables from:

$$W = R^{-1}Q = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

Multi-Moment Finite-Volume Method

- Homogeneous Conservation Equations

$$\frac{\partial Q}{\partial t}+\frac{\partial F(Q)}{\partial x}=0$$

- Spatially Differentiate the Conservation Equations

$$\frac{\partial}{\partial t}\left(\frac{\partial Q}{\partial x}\right)+\frac{\partial}{\partial x}\left(\frac{\partial F(Q)}{\partial x}\right)=0$$

- Apply Chain Rule to Fluxes (Characteristic Form)

$$\frac{\partial}{\partial t}\left(\frac{\partial Q}{\partial x}\right)+\frac{\partial}{\partial x}\left(\frac{\partial F}{\partial Q}\frac{\partial Q}{\partial x}\right)=0$$

- “Freeze” the Jacobian (Constant in time, Uniform in space)

$$\frac{\partial}{\partial t}\left(\frac{\partial Q}{\partial x}\right)+\frac{\partial F}{\partial Q}\frac{\partial}{\partial x}\left(\frac{\partial Q}{\partial x}\right)=0$$

Genuinely Multi-Dimensional: Bicharacteristics

- 2-D Characteristic Form

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial Q}\frac{\partial Q}{\partial x}+\frac{\partial H}{\partial Q}\frac{\partial Q}{\partial z}=0$$

- Diagonalize both Jacobians

$$\frac{\partial F}{\partial Q}=A_x=R_x\Lambda_x R_x^{-1} \qquad \frac{\partial H}{\partial Q}=A_z=R_z\Lambda_z R_z^{-1}$$

- Create a directional Jacobian

$$A(\theta)=\frac{\partial F}{\partial Q}\cos\theta+\frac{\partial H}{\partial Q}\sin\theta$$

- Diagonalize the directional Jacobian

$$A(\theta)=R(\theta)\Lambda(\theta)R^{-1}(\theta)$$

- Left-Multiply by $R^{-1}(\theta)$

$$R^{-1}(\theta)\frac{\partial Q}{\partial t}+R^{-1}(\theta)A_x\frac{\partial Q}{\partial x}+R^{-1}(\theta)A_z\frac{\partial Q}{\partial z}=0$$

- Insert $R(\theta)\,R^{-1}(\theta)$

$$R^{-1}(\theta)\frac{\partial Q}{\partial t}+R^{-1}(\theta)A_xR(\theta)R^{-1}(\theta)\frac{\partial Q}{\partial x}+R^{-1}(\theta)A_zR(\theta)R^{-1}(\theta)\frac{\partial Q}{\partial z}=0$$

Genuinely Multi-Dimensional: Bicharacteristics

$$R^{-1}(\theta)\frac{\partial Q}{\partial t}+R^{-1}(\theta)A_x R(\theta)R^{-1}(\theta)\frac{\partial Q}{\partial x}+R^{-1}(\theta)A_z R(\theta)R^{-1}(\theta)\frac{\partial Q}{\partial z}=0$$

- "Freeze" the Jacobian & Pull $R^{-1}(\theta)$ inside the derivatives

$$\frac{\partial W(\theta)}{\partial t}+B_x(\theta)\frac{\partial W(\theta)}{\partial x}+B_z(\theta)\frac{\partial W(\theta)}{\partial z}=0$$

$$B_x(\theta)=R^{-1}(\theta)A_x R(\theta)\qquad B_z(\theta)=R^{-1}(\theta)A_z R(\theta)\qquad W(\theta)=R^{-1}(\theta)Q$$

- Split B_x and B_z into a diagonal matrix and the remaining entries

$$B_x(\theta)=B_{x,D}(\theta)+B_x^{'}(\theta)\qquad B_z(\theta)=B_{z,D}(\theta)+B_z^{'}(\theta)$$

$$\frac{\partial W(\theta)}{\partial t}+B_{x,D}(\theta)\frac{\partial W(\theta)}{\partial x}+B_{z,D}(\theta)\frac{\partial W(\theta)}{\partial z}=S(\theta)$$

$$S(\theta)=-B_x^{'}(\theta)\frac{\partial W(\theta)}{\partial x}-B_z^{'}(\theta)\frac{\partial W(\theta)}{\partial z}$$

Genuinely Multi-Dimensional: Bicharacteristics

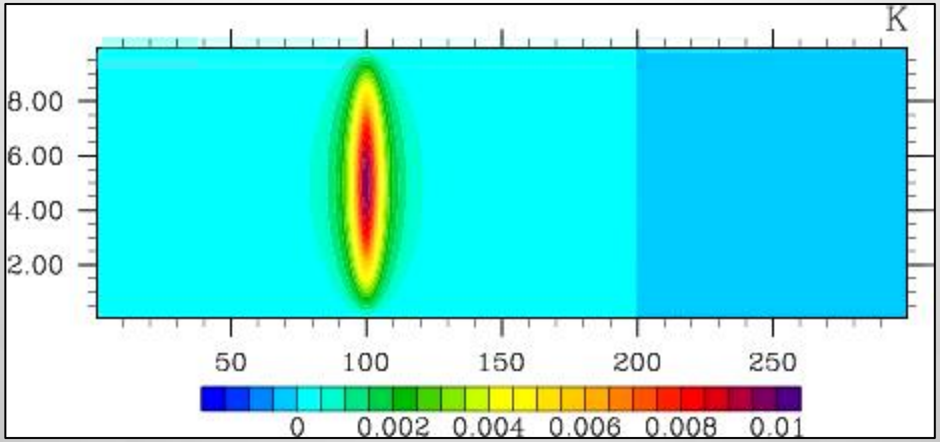
$$\frac{\partial W(\theta)}{\partial t} + B_{x,D}(\theta)\frac{\partial W(\theta)}{\partial x} + B_{z,D}(\theta)\frac{\partial W(\theta)}{\partial z} = S(\theta)$$

- Integrate in time $W_{P,n+1}(\theta) = W_{*,n}(\theta) + \int_{t_n}^{t_{n+1}} S(\theta)\,dt$
- Left-Multiply by R(θ) $Q_{P,n+1}(\theta) = R(\theta)W_{*,n}(\theta) + \int_{t_n}^{t_{n+1}} R(\theta)S(\theta)\,dt$
- Integrate in θ $Q_{P,n+1} = \frac{1}{2\pi}\int_0^{2\pi} R(\theta)W_{*,n}(\theta)\,d\theta + \frac{1}{2\pi}\int_0^{2\pi}\int_{t_n}^{t_{n+1}} R(\theta)S(\theta)\,dt\,d\theta$

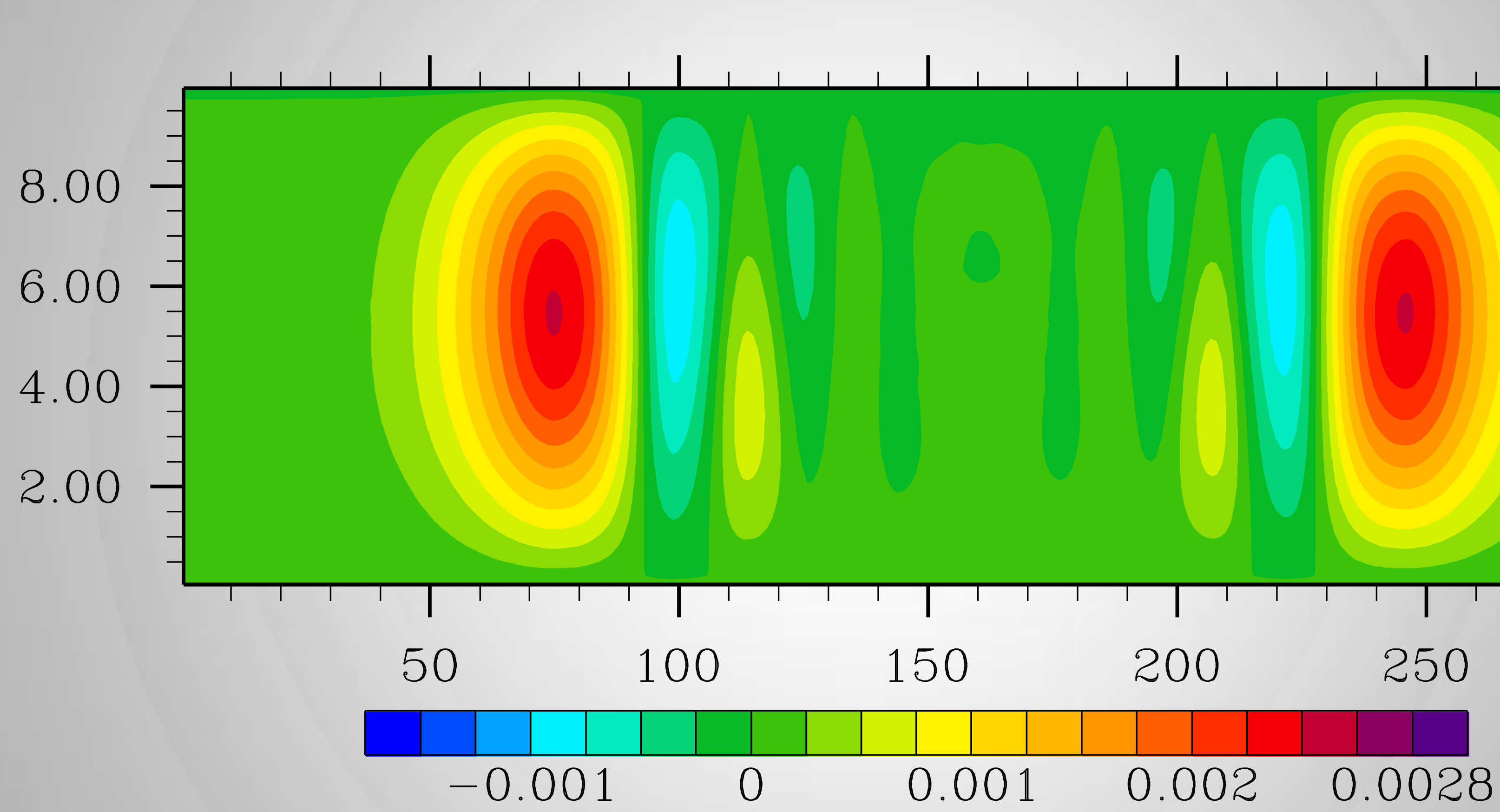
- Predicts state variables at a point in space and time
  - Takes into account full multidimensional nature of the characteristics
  - Contains a messy “source term” which must be integrated in time
  - Line integrals in θ easily handled with quadrature

NH-Scale Gravity Waves Test Case

- Initial Conditions (Skamarock & Klemp, 1994, MWR)
  - Constant Brunt Vaisala frequency ($10^{-2}\ s^{-1}$)
  - hydrostatic balance
  - 20 m/s horizontal wind
  - 10^{-2} °K potential temperature perturbation
- Simulated for 3,000 s
- Δx = 1,000 m , Δz = 100 m
- CFL=0.9 ($\Delta t \approx 0.25$ s)

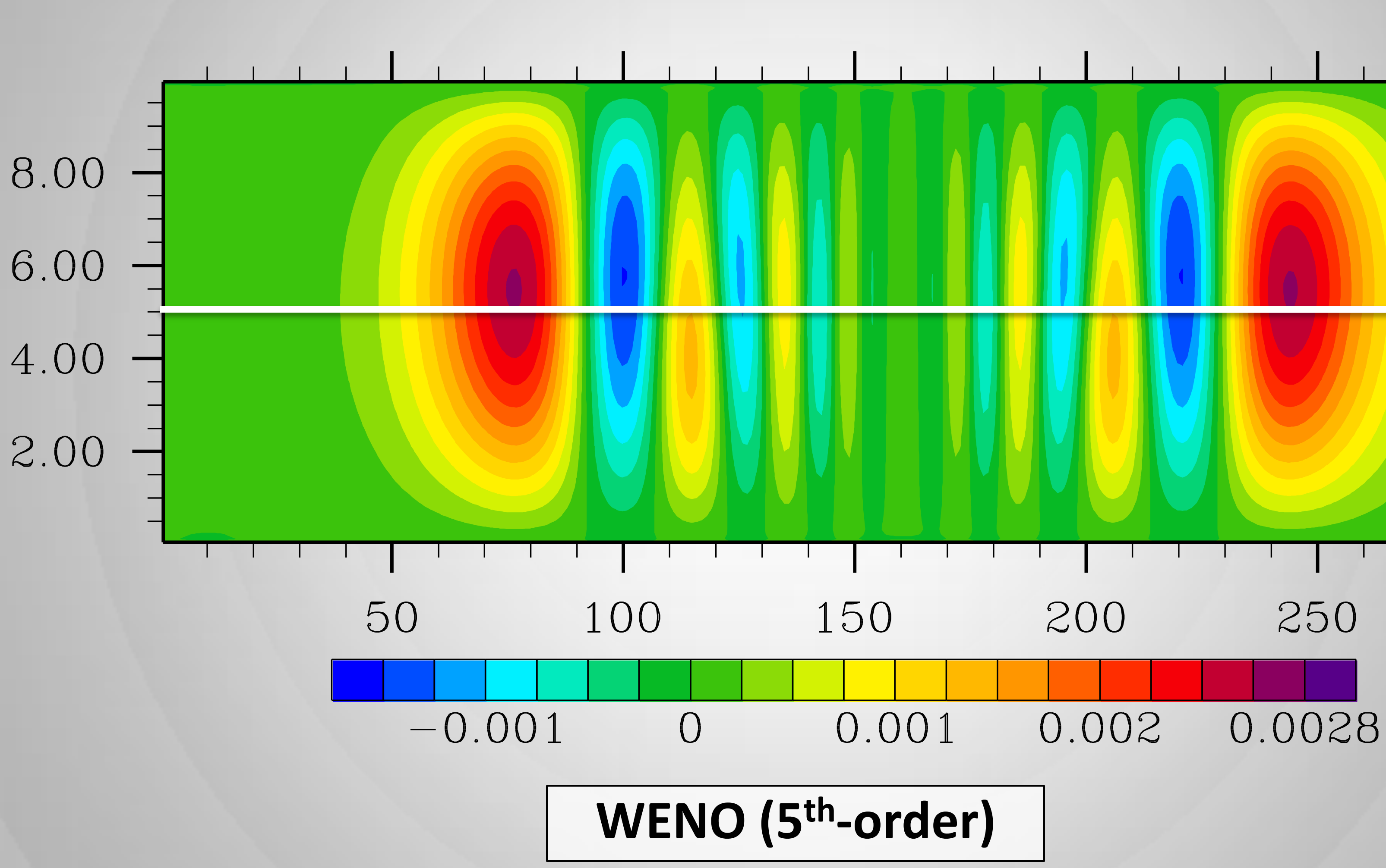


NH-Scale Gravity Waves Test Case

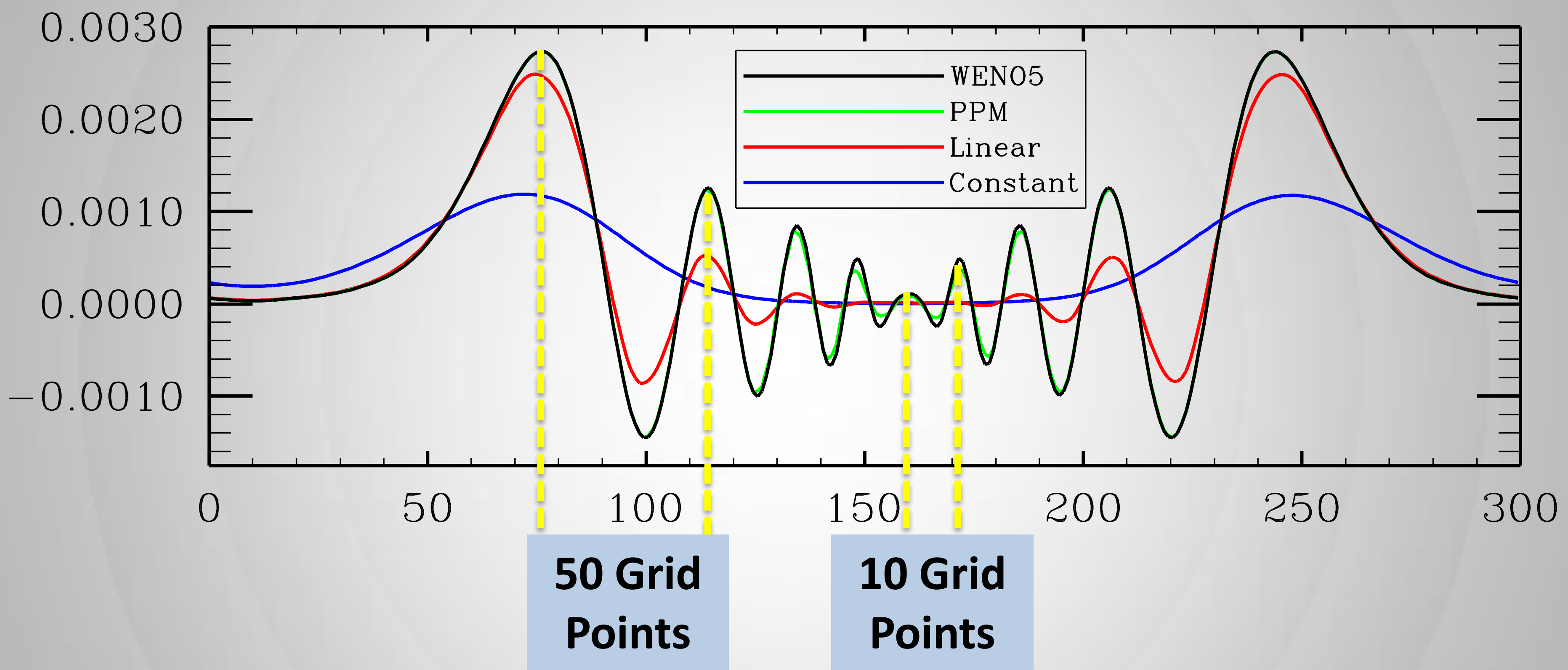


Linear (minmod)

NH-Scale Gravity Waves Test Case



NH-Scale Gravity Waves Test Case



Order of accuracy matters, even for well-resolved waves

It matters even more for poorly resolved waves