High order schemes in BATS-R-US: Is it OK to simplify them?

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Outline

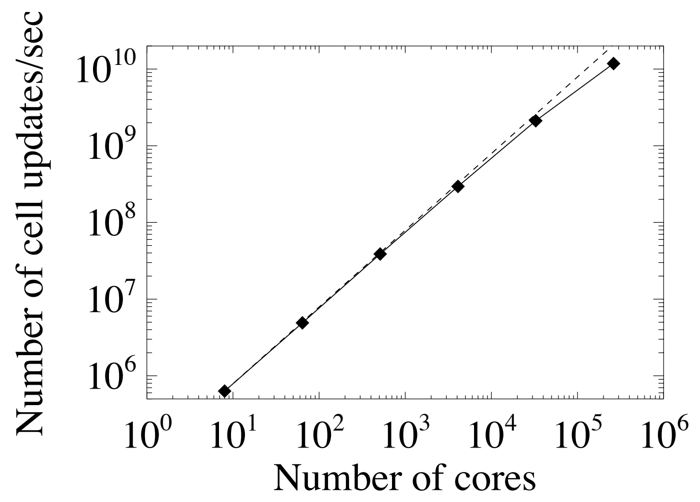
- Current BATS-R-US features and application areas
- Requirements for the high order scheme
- 4th order finite volume scheme
- 5th order monotonicity preserving scheme
- Some test results
- Some space physics applications
- Future work

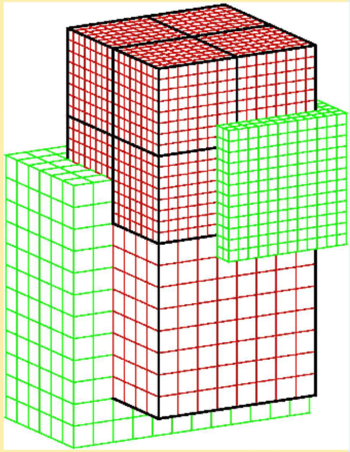
BATS-R-US

Block Adaptive Tree Solar-wind Roe Upwind Scheme

- **Physics**
  - Classical, semi-relativistic and Hall MHD
  - Multi-species, multi-fluid, anisotropic pressure
  - Radiation hydrodynamics multigroup diffusion
  - Multi-material, non-ideal equation of state
  - Solar wind turbulence, Alfven wave heating
- **Numerics**
  - Conservative finite-volume discretization
  - Parallel Block-Adaptive Tree Library (BATL)
  - Cartesian and generalized coordinates
  - Splitting the magnetic field into $B_0 + B_1$
  - Divergence B control: 8-wave, CT, projection, parabolic/hyperbolic
  - Numerical fluxes: Rusanov, AW, HLLE, HLLD, Roe
  - Explicit, point-implicit, semi-implicit, fully implicit time stepping
  - Up to 4th order accurate in time and 5th order in space
- **Applications**
  - Heliosphere, sun, planets, moons, comets, HEDP experiments
- **100,000+ lines of Fortran 90 code with MPI parallelization**

Parallel scaling from 8 to 262,144 cores on Cray Jaguar. 40,960 grid cells per core.





Requirements for High Order Schemes

- **We want a high order scheme that**
  - Is only moderately more expensive than the 2nd order TVD schemes.
    - Factor of 10 or even slower would not be very useful…
  - Can handle shock waves and other discontinuities.
    - Robust and does not generate spurious oscillations.
  - Can work for a variety of equations.
    - Does not require generation of equations for higher moments.
  - Can work in non-Cartesian coordinates.
  - Can work reasonably well together with AMR.
    - We may not have fully high order AMR scheme right away.
  - Does not require a complete rewrite of BATS-R-US.
- **Selected schemes (influenced by Mignone et al 2010)**
  - 4th order finite volume (FIVOL4) scheme by McCorquodale and Colella
  - 5th order monotonicity preserving (MP5) scheme by Suresh and Huynh

FIVOL4

- **The algorithm (on uniform Cartesian grid) requiring 5 ghost cells**
  - ✓ Store cell averages of conservative variables $\langle U \rangle_i$
  - ✓ Convert to cell center values $U_i = \langle U \rangle_i - \Delta x^2/24\ U_{xx}$
  - ✓ Convert to cell center primitive variables W_i
  - ✓ Convert to cell averaged primitive variables $\langle W \rangle_i = W_i + \Delta x^2/24\ W_{xx}$
  - ✓ Use 4th order accurate (PPM-like) limiter to get $\langle W \rangle^{L,R}_{i+1/2}$
  - ✓ Convert to 4th order accurate face center values $W^{L,R}_{i+1/2}$
  - ✓ Apply some Riemann solver to get face center flux $F_{i+1/2}$
  - ✓ Convert to face averaged flux $\langle F \rangle_{i+1/2}$
  - ✓ Update $\langle U \rangle_i$
- **RK4 in time**

2 AMR levels, 1024 x 256 cells effective resolution
from McCorquodale and Colella 2011

There is more …

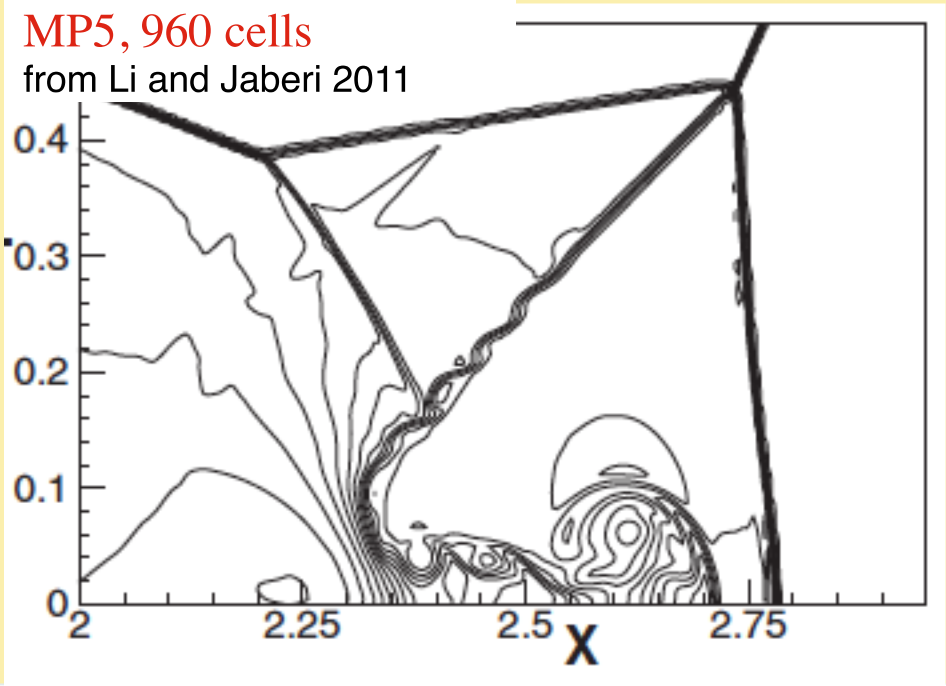
- **The algorithm (on uniform Cartesian grid) requiring 5 ghost cells**
  - ✓ Store cell averages of conservative variables $\langle U \rangle_i$
  - ✓ Convert to cell center values $U_i = \langle U \rangle_i - \Delta x^2/24\ U_{xx}$
  - ✓ Convert to cell center primitive variables W_i
  - ✓ Convert to cell averaged primitive variables $\langle W \rangle_I = W_i + \Delta x^2/24\ W_{xx}$
  - ✓ Use 4th order accurate (PPM-like) limiter to get $\langle W \rangle^{L,R}_{i+1/2}$
  - ✓ Convert to 4th order accurate face center values $W^{L,R}_{i+1/2}$
  - ✓ Apply some Riemann solver to get face center flux $F_{i+1/2}$
  - ✓ Convert to face averaged flux $\langle F \rangle_{i+1/2}$
  - ✓ Update $\langle U \rangle_i$
  - ➢ Source terms should also be based on point values and cell averaged
  - ✓ Apply shock flattening for strong shocks
  - ➢ Apply artificial viscosity to remove short wave length oscillations

There is less …

- **Simplified algorithm requiring 3 ghost cells**
  - ✓ Store cell center values of conservative variables U_i
  - ✓ Convert to cell center primitive variables W_i
  - ✓ Use almost 4th order accurate (PPM-like) limiter to get $W^{L,R}_{i+1/2}$
  - ✓ Apply some Riemann solver to get face center flux $F_{i+1/2}$
  - ✓ Update U_i
  - ✓ Source terms are added point-wise
  - ✓ Apply shock flattening for strong shocks
  - ➢ Apply artificial viscosity to remove short wave length oscillations
- **An almost 4th order finite difference scheme for linear equations**

MP5

- The algorithm (on uniform Cartesian grid) requiring **3 ghost cells**
  - ✓ Store cell center values of conservative variables U_i
  - ➢ Convert to characteristic fluxes $\hat{F}_i = L^{Roe}_{i+1/2} F_i$
  - ✓ Calculate cell centered Lax-Friedrichs split fluxes $\hat{F}^{\pm}_i = (\hat{F}_i \pm c_{\max} \hat{U}_i)/2$
  - ✓ Interpolate to 5th order accurate limited characteristic face flux $\hat{F}^{\pm}_{i+1/2}$
  - ➢ Convert to conservative face flux $F_{i+1/2} = R^{Roe}_{i+1/2}(\hat{F}^{+}_{i+1/2} + \hat{F}^{-}_{i+1/2})$
  - ✓ Update U_i
- RK3 in time



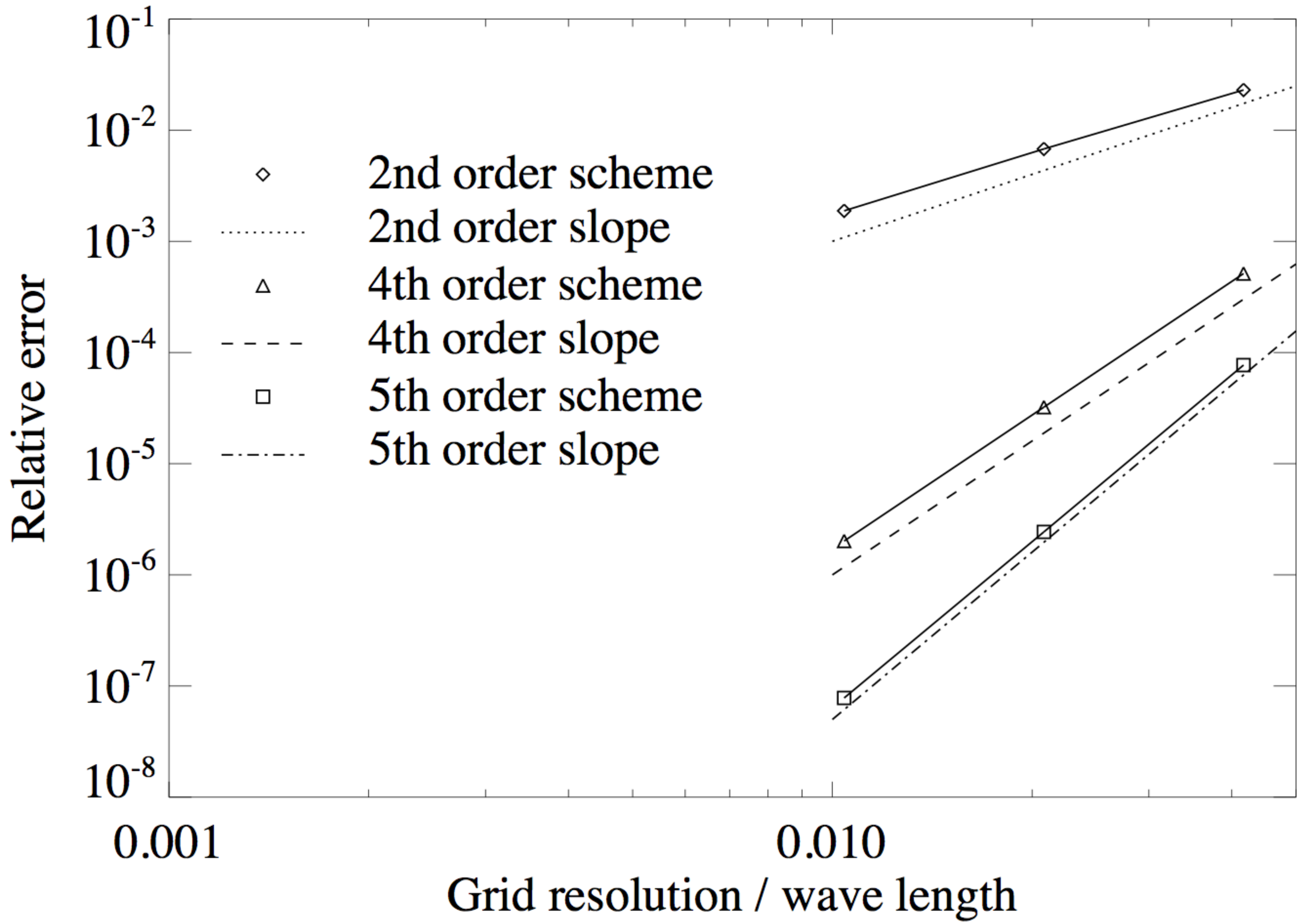
Simplified MP5

- **The algorithm (on uniform Cartesian grid) requiring 3 ghost cells**
  - ✓ Store cell center values of conservative variables U_i
  - ✓ Interpolate to 5th order accurate limited face values $U_{i+1/2}^{L,R}$
  - ✓ Calculate face flux (Rusanov, HLL)
  - ✓ Update U_i
- **This is only 5th order accurate for linear problems**
  - ... but it is really simple and easy to implement into our code ...
  - ... no conversion to and from characteristic domain ...

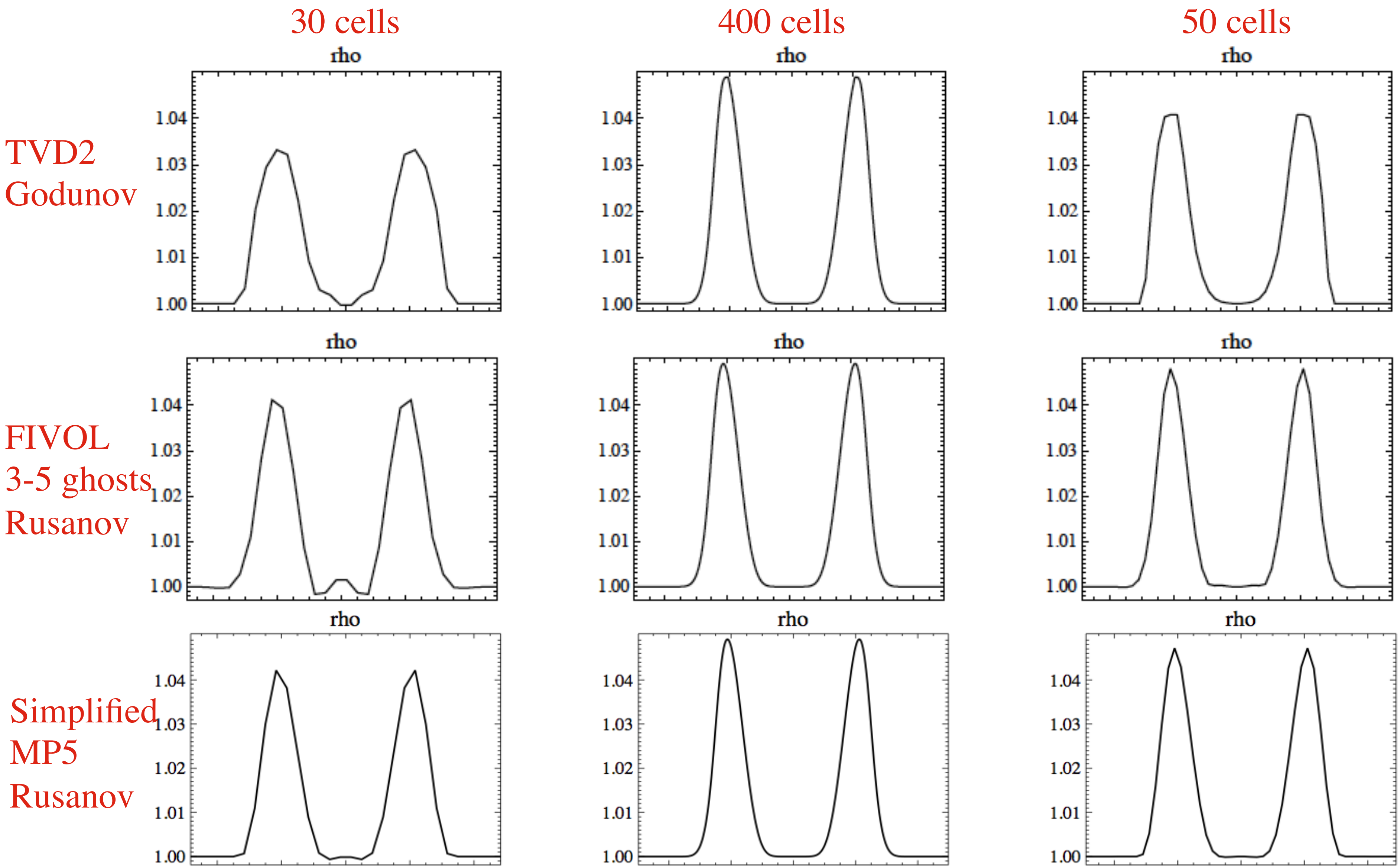
Verification tests

- Advection of a Gaussian profile in 1D and 2D: linear scalar equation
- Alfven waves in 1D and 2D: linear system of equations
- Gaussian pressure pulse in 1D and 2D: non-linear system of equations
- Advection of a tophat in 1D and 2D: non-compressive discontinuity
- Shu-Osher shock tube problem in 1D: compressive discontinuity
- Advection on AMR grid: effects of 2nd order scheme at res. change
- Advection on cylindrical and spherical grids: non-Cartesian effects

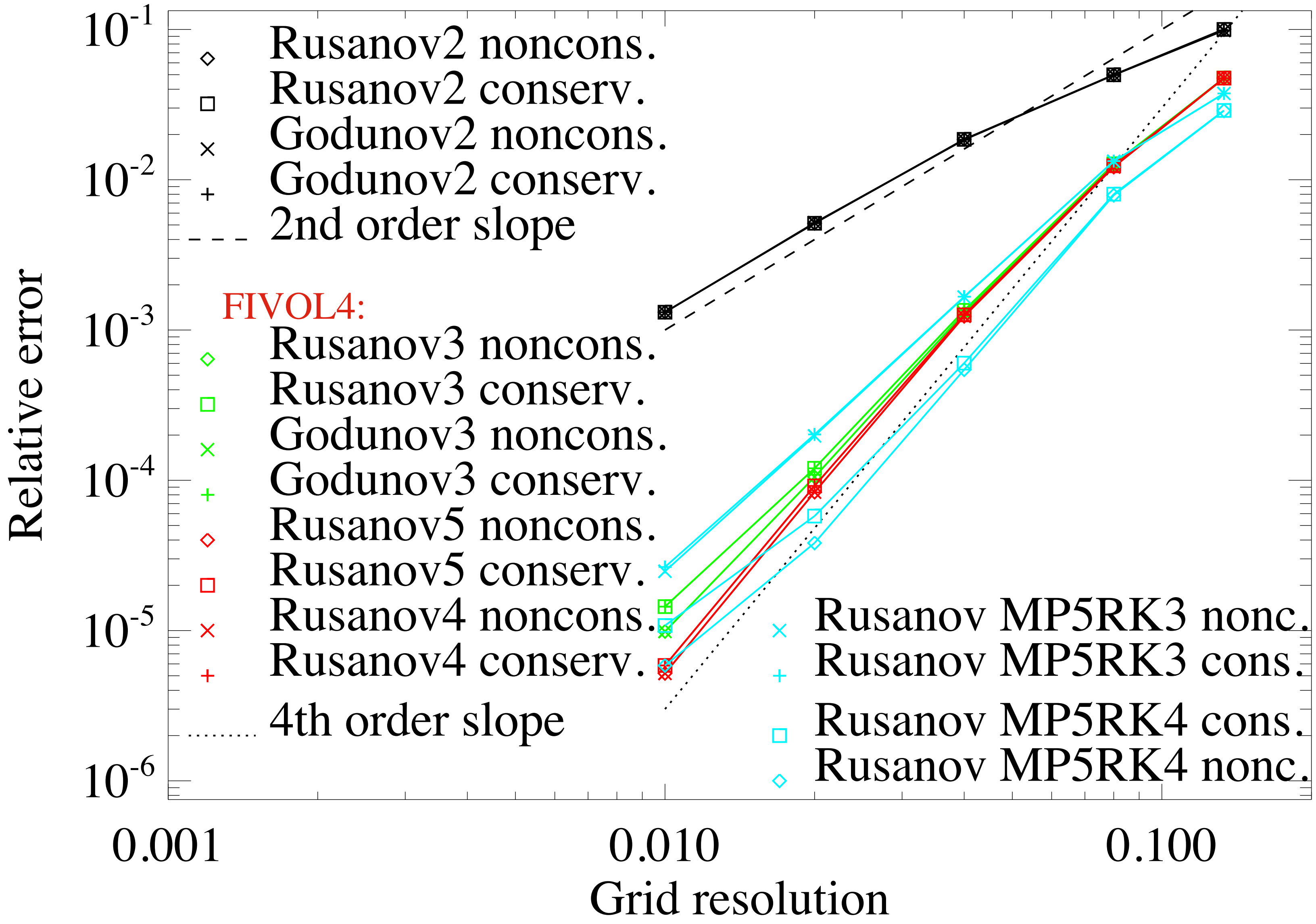
Circularly polarized Alfven waves in 2D



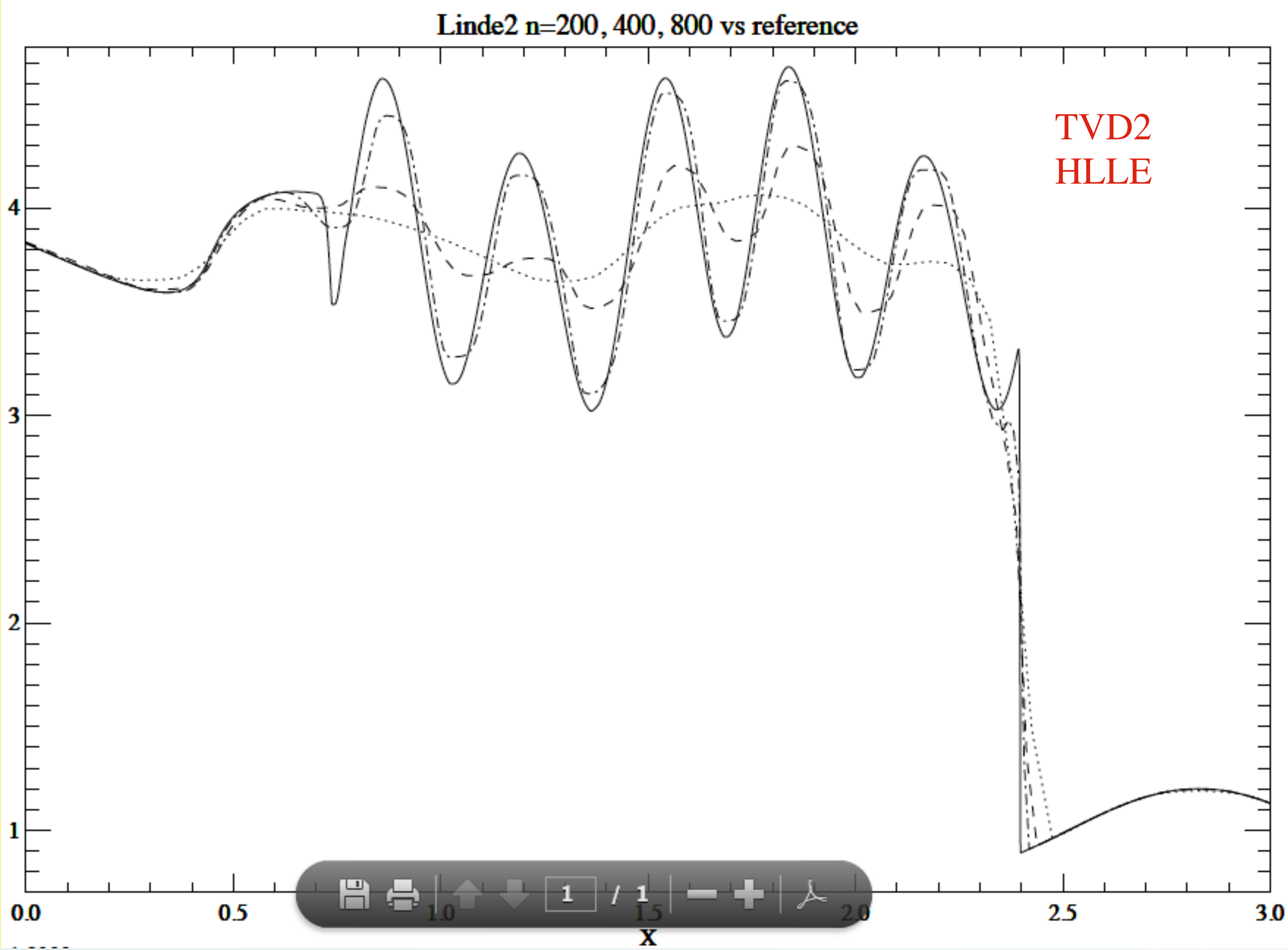
Gaussian pressure pulse in 1D



Gaussian pressure pulse in 1D



Shu-Osher test in 1D



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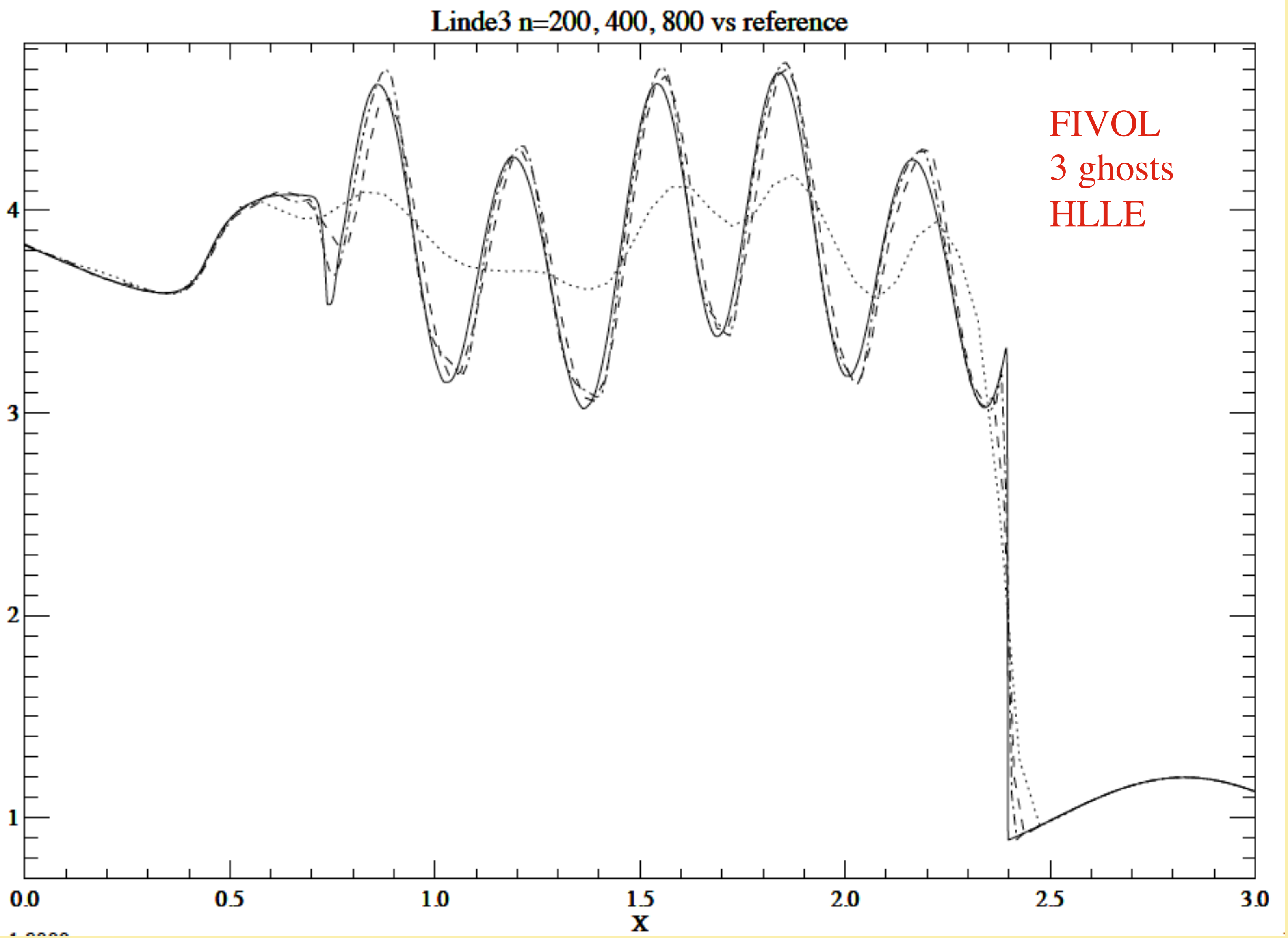

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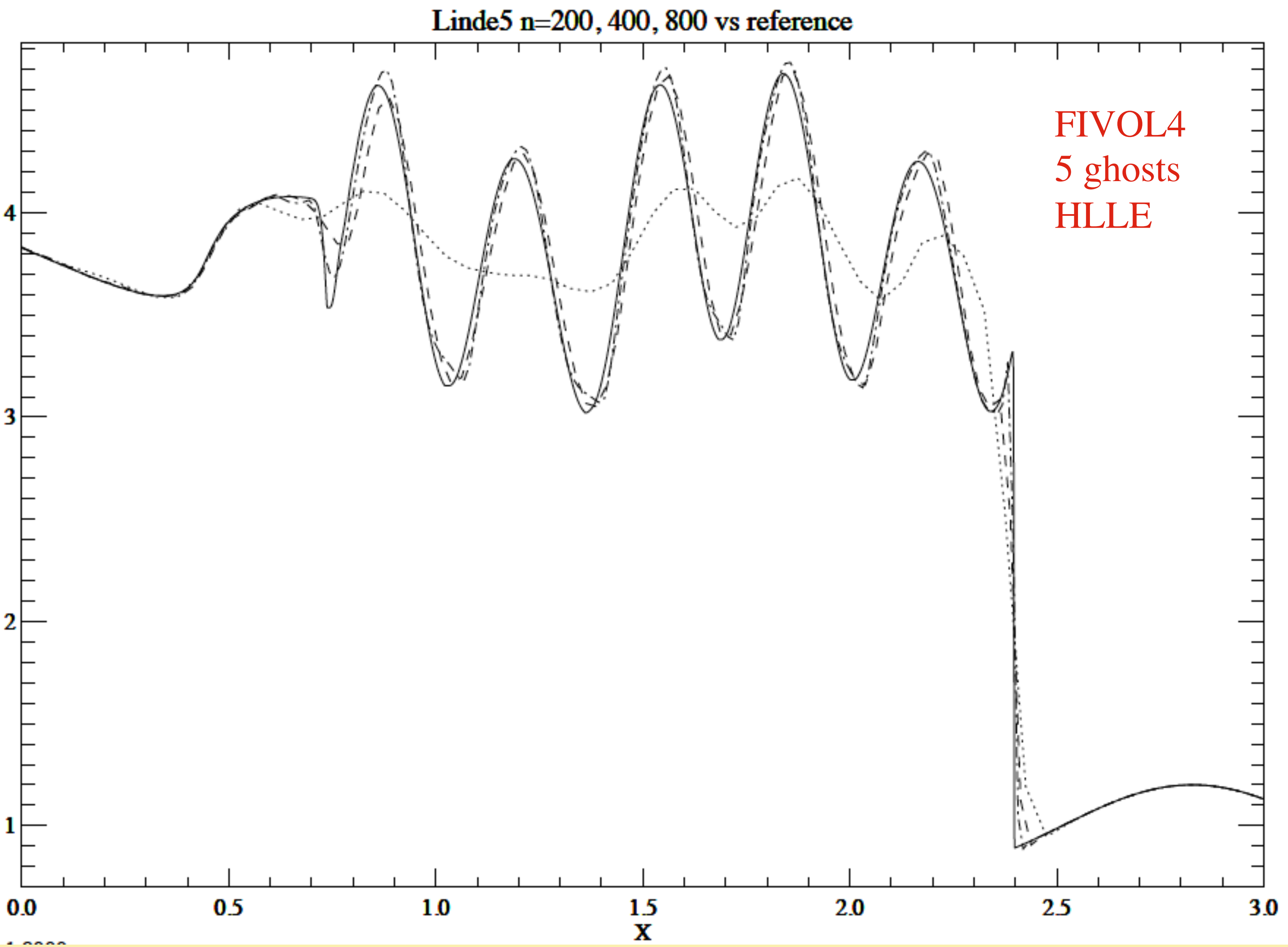

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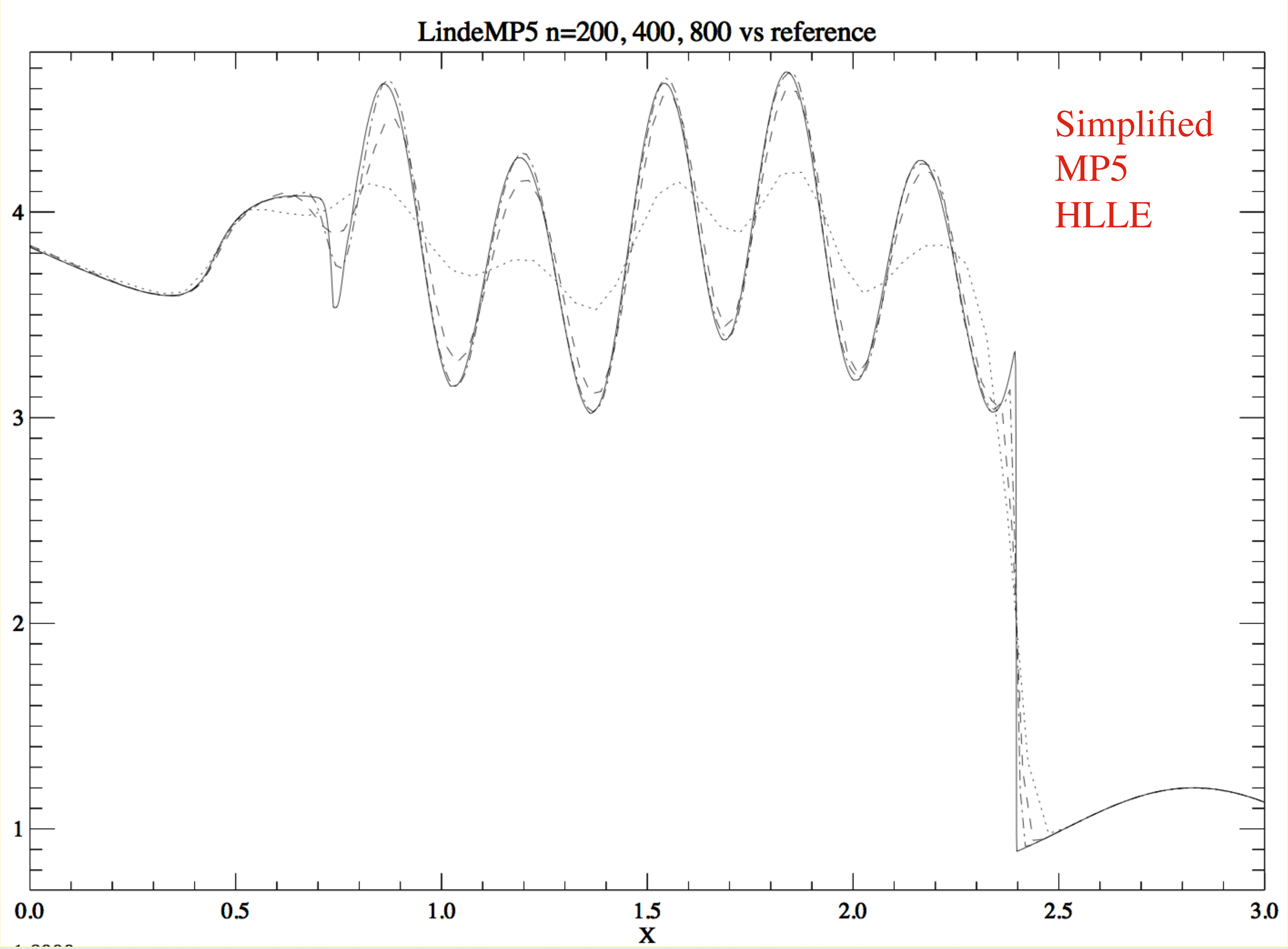
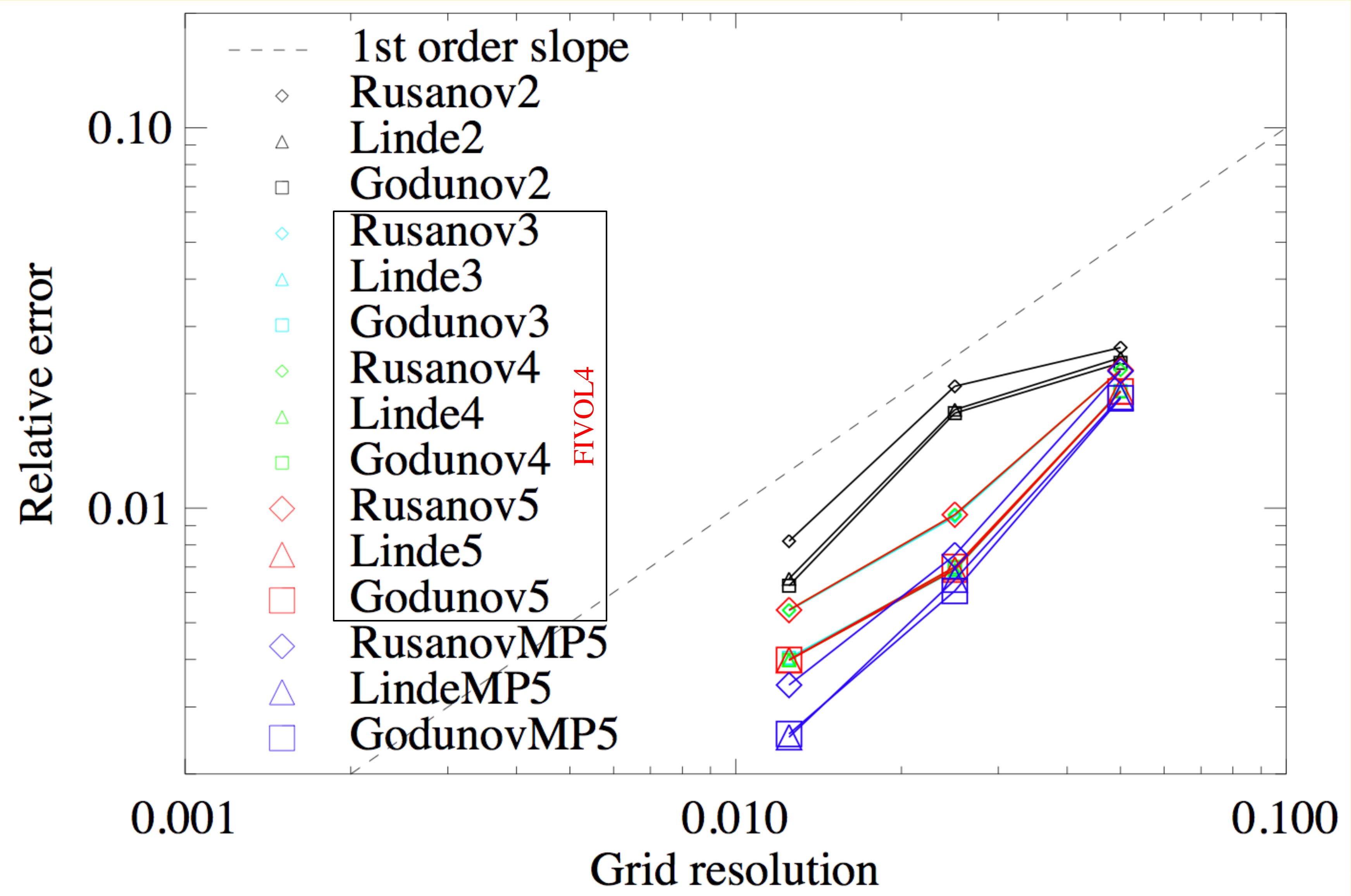


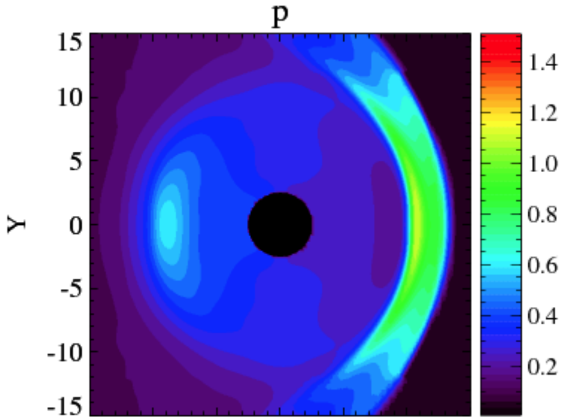
Shu-Osher test in 1D



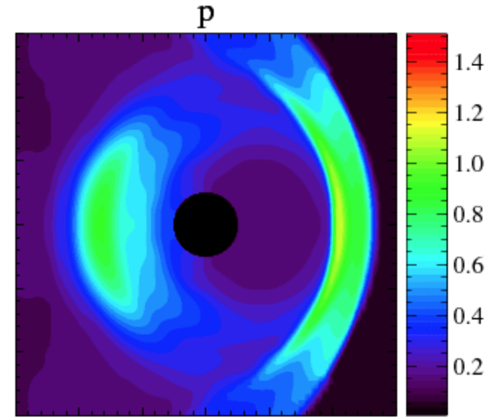
Magnetosphere Simulations

- **Pure MHD with split magnetic field and an inner boundary**
  - Varied resolution from 1/4 to 1/16 R_E within $-10R_E < x, y, z < 10R_E$
  - The new high order schemes produce negative pressure and density
    - Implemented floor values for pressure and density
    - Modified the MP5 limiter to avoid negative pressure and density
  - Empty regions above poles
    - Tried outflow: no improvement
    - Tried non-uniform resistivity: not better
    - Added uniform resistivity: somewhat better
- **Coupled runs with inner magnetosphere**
  - Large velocities in the closed magnetic field region
    - Unresolved problem
- **Any good news?**

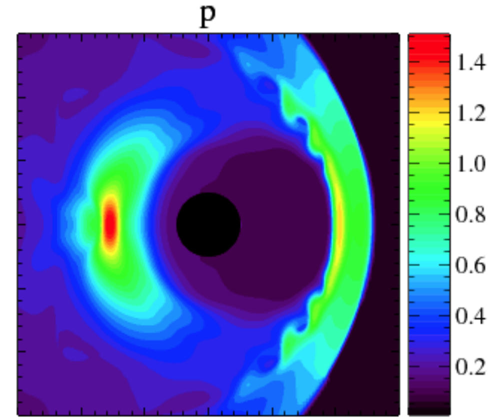
Solar wind: n=5/cc, u_x=400km/s, B_z= -5nT
Magnetic diffusion: 10^{11} m^2/s



TVD 1/4 R_E

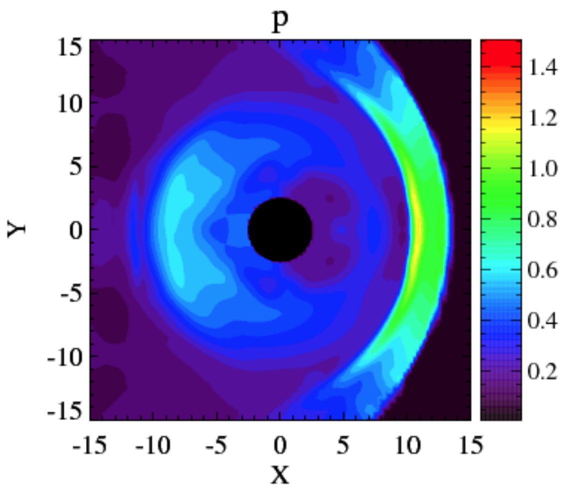


TVD 1/8 R_E

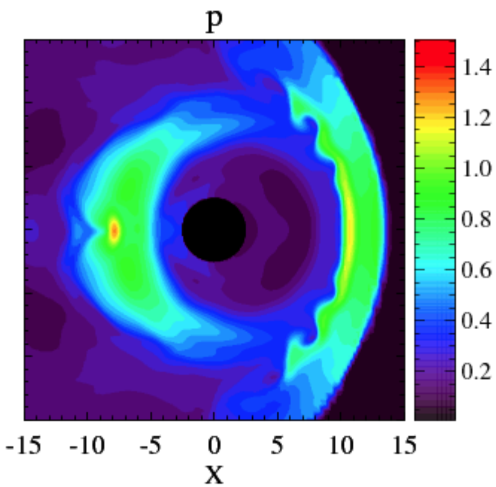


TVD 1/16 R_E

MP5 1/4 R_E



MP5 1/8 R_E



Heliospheric Simulations

- **Split magnetic field, Alfven wave turbulence, heat conduction, steady state solution in rotating frame, highly stretched spherical grid**
  - The new high order schemes produce negative pressure and density
    - Apply floor values for pressure and density
    - Switch to MP5 after 10,000 iterations with the TVD scheme
    - Still crashes, but only after many (~70,000) iterations
- **Any good news?**

Center for Space Environment Modeling
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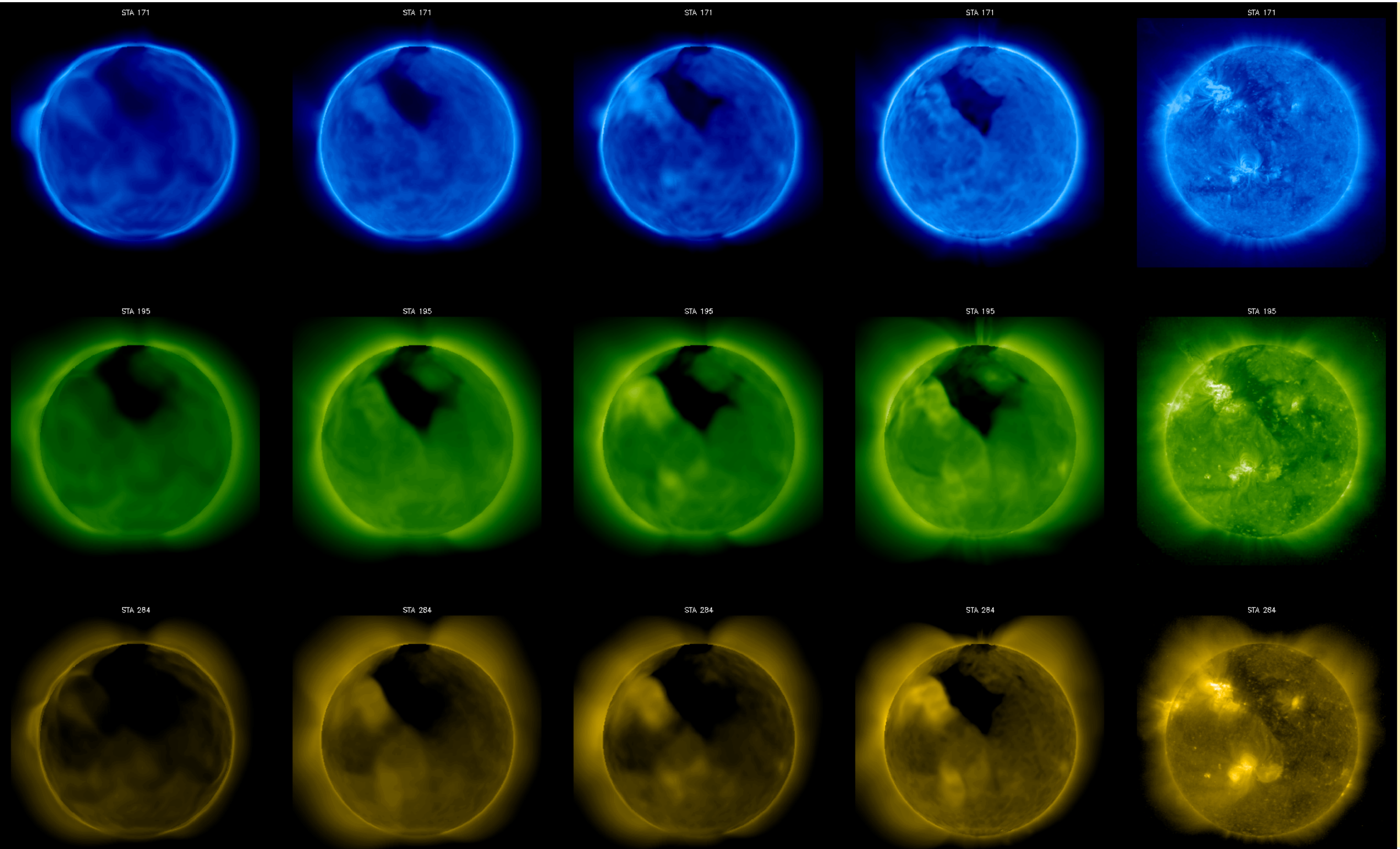
Space Weather Modeling Framework

Line-of-Sight Integrated Images
Stereo A, March 7 2011

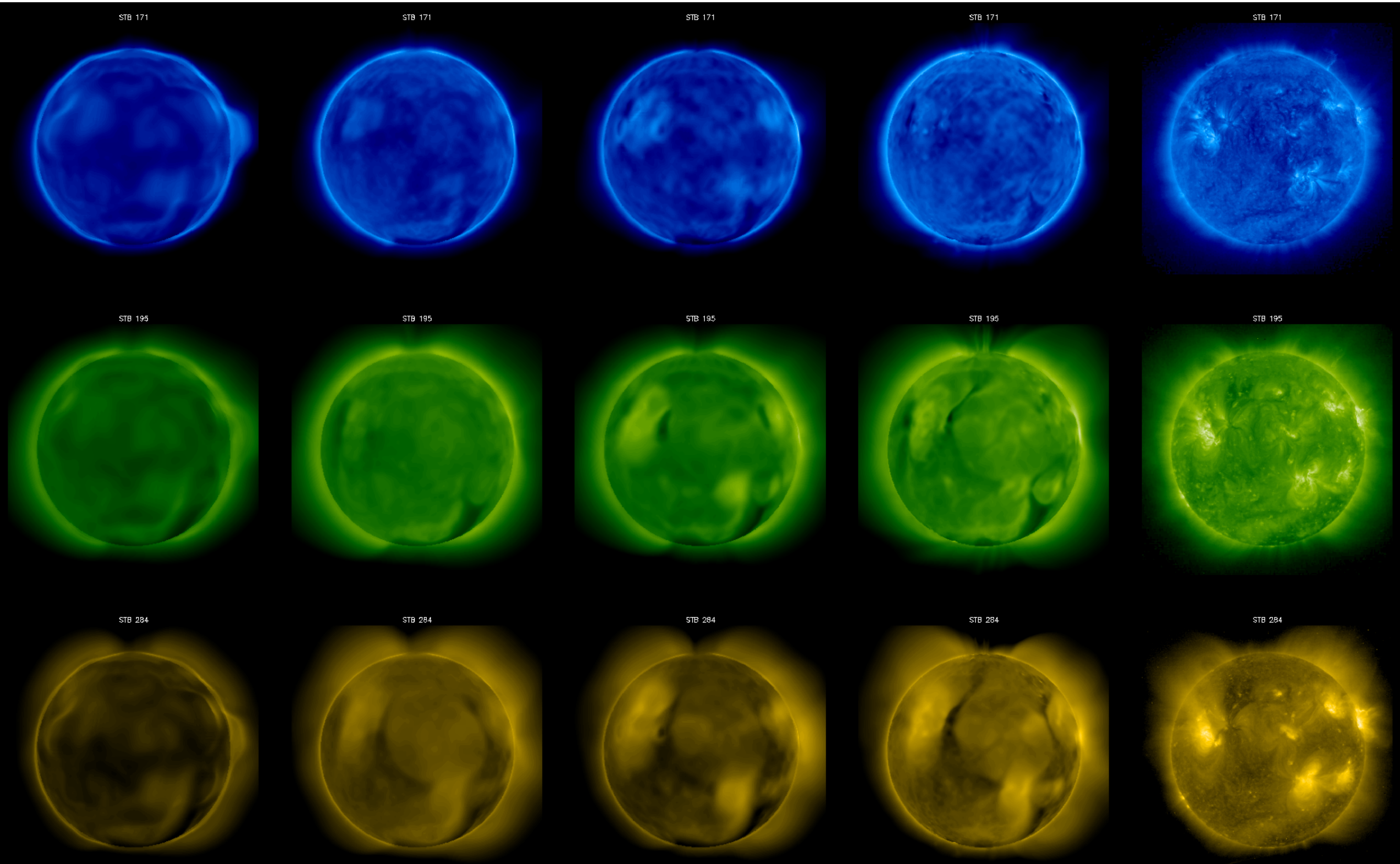
TVD coarse	TVD fine	MP5 coarse	MP5 fine	Observation



Center for Space Environment Modeling
Space Weather Modeling Framework

Line-of-Sight Integrated Images
Stereo B, March 7 2011

TVD coarse | TVD fine | MP5 coarse | MP5 fine | Observation



Summary

- **BATS-R-US (BATL) now works with arbitrary number of ghost cells**
- **Various Runge-Kutta time stepping schemes (RK2, RK3, RK4)**
- **FIVOL4 is implemented for uniform Cartesian grids**
  - Simplified version requires 3 ghost cells only
- **MP5 is implemented for interpolating primitive variables or fluxes**
- **Verification tests suggest that the simplifications have little impact**
- **Magnetosphere simulations**
  - Problems with positivity, unexpected features
  - Promising results for KH instability: similar as TVD on twice finer grid
- **Heliosphere simulations**
  - Robustness issues
  - Promising results for LOS images: better than TVD on twice finer grid
- **Plan: CWENO5 with finite difference approach, AMR, non-Cartesian…**