# Numerical Approaches to Fluidand Magnetohydrodyanamics in Astrophysics

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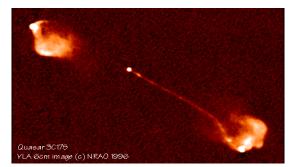


- I. Plasma as fluids, validity of MHD;
- II. The linear advection equation: concepts & discretizations;
- III. Nonlinear hyperbolic PDE: shocks and expansion waves;
- IV. Finite Volume Methods: state of the art Godunov-type codes;
- V. Beyond MHD: extending current computational models.

#### I. PLASMAS AS FLUIDS

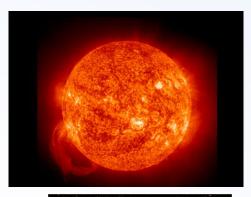
## **Observational Evidence**

- It is estimated that more than 99.9 % of matter in the Universe exists in the form of <u>plasma</u>;
- A *plasma* is a ionized gas where charged particles interact via electromagnetic forces (electric and magnetic fields);
- Examples include stars, nebulae, galaxies, supernovae, interstellar/galactic medium, jets, accretion disks, etc..
- Our knowledge limited by what we can actually observe → emitting plasma.











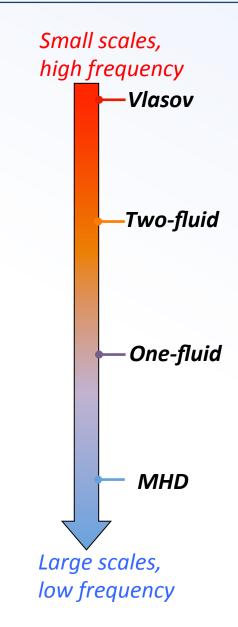


# From Kinetic to Fluid to MHD

 <u>Vlasov / Fokker Plank</u> describes the time evolution, in phase space, of the plasma distribution function f(x,v,t):

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q}{mc} \left( \mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right) \cdot \nabla_{\mathbf{v}} f = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

- <u>Two-fluid model</u> (ions & electrons) derived by integrating  $v^n f(\mathbf{x}, \mathbf{v}, t)$  over velocity space and taking moments of increasingly higher order.
- A <u>one fluid model</u> is derived by proper average of the ions and electrons fluid equations.
- <u>Magnetohydrodynamics</u> (MHD) is a further simplification of the one fluid model.



# Validity of Fluid approximations

- The fluid approach treats the system as a <u>continuous medium</u> and considering the dynamics of a small volume of the fluid.
- Meaningful to model length <u>scales much greater than mean free path</u> or individual particle trajectories.
- "Fluid element": small enough that any macroscopic quantity has a negligible variation across its dimension but large enough to contain many particles and so to be insensitive to particle fluctuations.
- Fluid equations involve only <u>moments</u> of the distribution function relating mean quantities. Knowledge of f(x,v,t) is not needed<sup>\*</sup>.
- Still: taking moments of the Vlasov equation lead to the appearance of a next higher order moment → "loose end" → <u>Closure</u>.

## Magetohydrodynamics: Assumptions

- Ideal MHD describes an electrically conducting single fluid, assuming:
  - low frequency  $\omega \ll \omega_p$ ,  $\omega \ll \omega_c$ ,  $\omega \ll \nu_{pe}$ ,  $\omega \ll \nu_{ep}$

- large scales 
$$L \gg \frac{c}{\omega_p}$$
,  $L \gg R_c$ ,  $L \gg \lambda_{mfp}$ ,

- Ignores electron mass and finite Larmor radius effects;
- Assume plasma is *strongly collisional*  $\rightarrow$  L.T.E., isotropy;
- Fields and fluid fluctuate on the same time and length scales;
- Neglect charge separation, electric force and displacement current.

## Ideal MHD at Last

- MHD suitable for describing plasma at large scales;
- $J = \frac{c}{4\pi} \nabla \times B \quad (Ampere)$ Good first approximation to much of the physics even when some of the conditions are not met.

$$7 \cdot \mathbf{B} = 0$$
 (Divergence - free)

- Draw some intuitive conclusions concerning plasma behavior without solving the equations in detail.
- Fluid equations are <u>hyperbolic</u> conservation laws.

## (Special) Relativistic Ideal MHD

• Special relativistic MHD equations:

$$\frac{\partial(\rho\gamma)}{\partial t} + \nabla \cdot (\rho\gamma \mathbf{v}) = 0,$$
  
$$\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot [w\gamma^2 \mathbf{v}\mathbf{v} - \mathbf{B}\mathbf{B} - \mathbf{E}\mathbf{E}] + \nabla p_t = 0,$$
  
$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) = 0,$$
  
$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathbf{m} - \rho\gamma \mathbf{v}) = 0,$$
  
$$\mathcal{E} = w\gamma^2 - p + \frac{\mathbf{B}^2 + \mathbf{E}^2}{2} - \rho\gamma$$

- Relativistic effects:
  - Bulk motion:  $v \approx c$ ;
  - Strongly magnetized rarefied plasmas:  $V_A \approx c$ ;
  - Extremely hot plasmas:  $kT/m \approx c^2$ .
- Both MHD and relaticistic MHD are <u>nonlinear systems of hyperbolic PDE</u>.

#### **II. THE LINEAR ADVECTION EQUATION:** CONCEPTS AND DISCRETIZATIONS

# **The Advection Equation: Theory**

• First order partial differential equation (PDE) in (x,t):

$$rac{\partial U(x,t)}{\partial t} + a rac{\partial U(x,t)}{\partial x} = 0$$

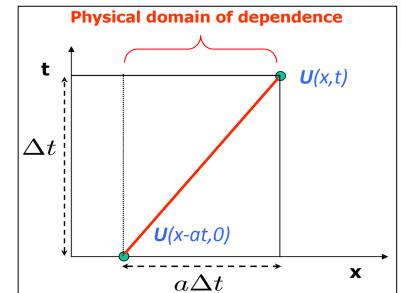
Hyperbolic PDE: information propagates across domain at <u>finite speed</u>
 → method of characteristics

 $\frac{dx}{dt} = a$ 

• Characteristic curves satisfy:

 $\frac{dU}{dt} = \frac{\partial U}{\partial t} + \frac{dx}{dt}\frac{\partial U}{\partial x} = 0$ 

 $\rightarrow$  The solution is constant along characteristic curves.

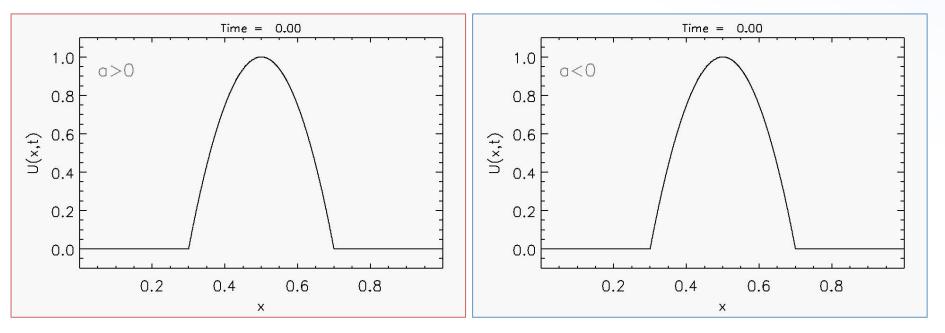


#### **The Advection Equation: Theory**

 for constant *a*: the characteristics are straight parallel lines and the solution to the PDE is a uniform shift of the initial profile:

$$U(x,t) = U(x - at, 0)$$

• The solution shifts to the right (for a > 0) or to the left (a < 0):



## **Discretization: the FTCS Scheme**

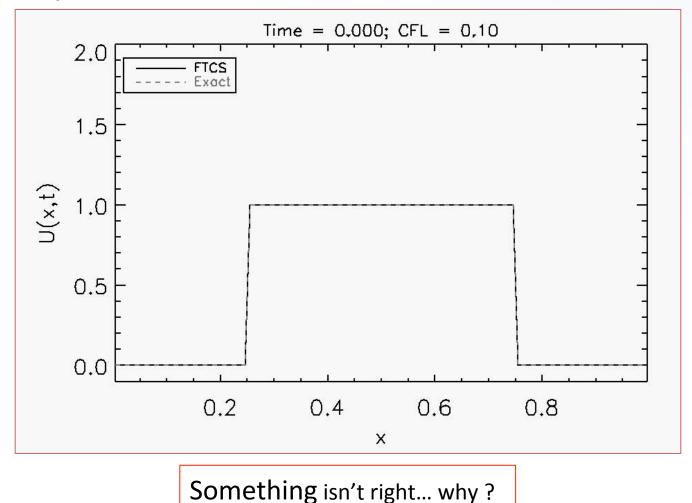
- Consider our model PDE  $\frac{\partial U(x,t)}{\partial t} + a \frac{\partial U(x,t)}{\partial x} = 0$
- Forward derivative in time:  $\frac{\partial U(x,t)}{\partial t} \approx \frac{U_i^{n+1} U_i^n}{\Delta t} + O(\Delta t)$ Centered derivative in space:  $\frac{\partial U(x,t)}{\partial x} \approx \frac{U_{i+1}^n U_{i-1}^n}{2\Delta x} + O(\Delta x^2)$ •
- Putting all together and solving with respect to  $U^{n+1}$  gives

$$U_{i}^{n+1} = U_{i}^{n} - \frac{C}{2} \left( U_{i+1}^{n} - U_{i-1}^{n} \right)$$

where  $C = a \Delta t / \Delta x$  is the Courant-Friedrichs-Lewy (CFL) number.

- We call this method *FTCS* for <u>Forward in Time</u>, <u>Centered in Space</u>. ٠
- It is an explicit method. ٠

• At t=0, the *initial condition* is a square pulse with periodic boundary conditions:



## FTCS: von Neumann Stability Analysis

- Let's perform an analysis of *FTCS* by expressing the solution as a Fourier series.
- Since the equation is linear, we only examine the behavior of a single mode. Consider a trial solution of the form:

 $U_i^n = A^n e^{Ii\theta} \,, \quad \theta = k\Delta x$ 

- Plugging in the difference formula:  $\frac{A^{n+1}}{A^n} = 1 \frac{C}{2} \left( e^{I\theta} e^{-I\theta} \right)$  $\implies \qquad \left| \frac{A^{n+1}}{A^n} \right|^2 = 1 + C^2 \sin^2 \theta \ge 1$
- Indipendently of the CFL number, all Fourier modes increase in magnitude as time advances.
- This method is <u>unconditionally unstable!</u>

## Forward in Time, Backward in Space

- Let's try a difference approach. Consider the backward formula for the spatial derivative:
  - $\frac{\partial U}{\partial x} \approx \frac{U_i^n U_{i-1}^n}{\Delta x} + O(\Delta x) \quad \Longrightarrow$
- The resulting scheme is called FTBS:

$$U_i^{n+1} = U_i^n - C\left(U_i^n - U_{i-1}^n\right)$$

 Apply von Neumann stability analysis on the resulting discretized equation:

$$\left|\frac{A^{n+1}}{A^n}\right|^2 = 1 - 2C(1-C)(1-\cos\theta)$$

• <u>Stability</u> demands

$$\left|\frac{A^{n+1}}{A^n}\right| \le 1 \quad \Longrightarrow \quad 2C(1-C) \ge 0$$

- for a < 0 the method is <u>unstable</u>, but
- for a > 0 the method is <u>stable</u> when  $0 \le C = a \Delta t / \Delta x \le 1$ .

## Forward in Time, Forward in Space

• Repeating the same argument for the forward derivative

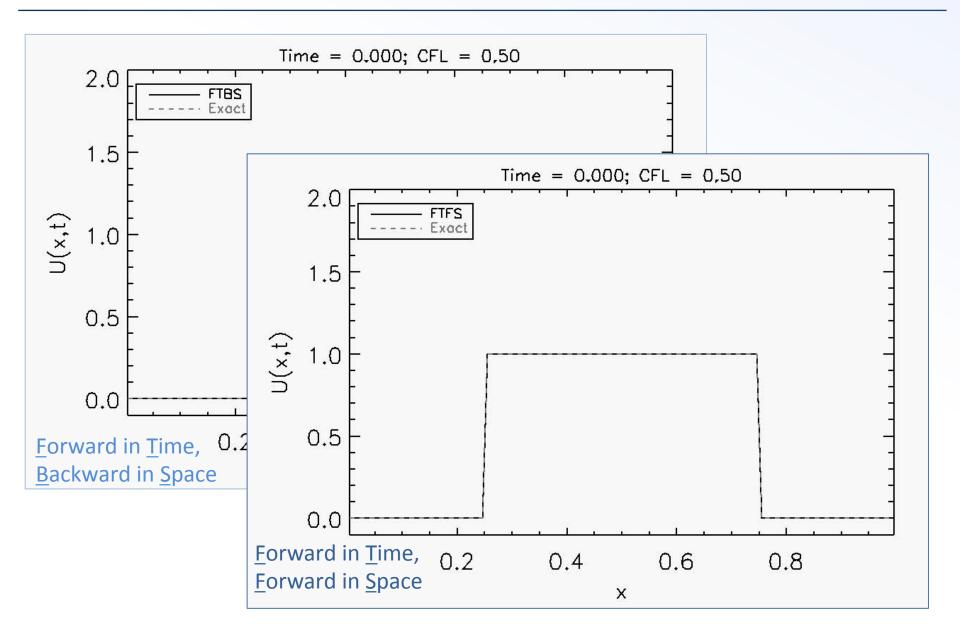
$$\frac{\partial U}{\partial x} \approx \frac{U_{i+1}^n - U_i^n}{\Delta x} + O(\Delta x) \quad \Longrightarrow \quad \left[ U_i^{n+1} = U_i^n - C\left(U_{i+1}^n - U_i^n\right) \right]$$

• The resulting scheme is called FTFS:

• Apply stability analysis yields 
$$\left|\frac{A^{n+1}}{A^n}\right|^2 = 1 + 2C(1-C)(1-\cos\theta)$$

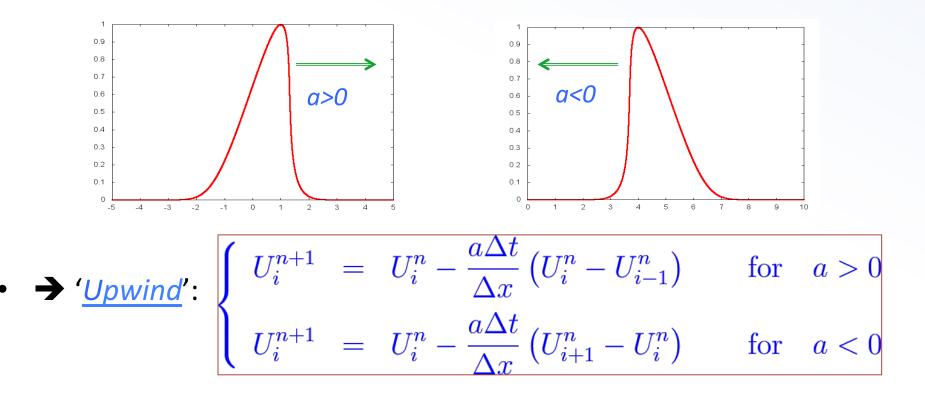
- If *a* > *0* the method will always be <u>unstable</u>
- However, if a < 0 and  $-1 \le C = a \Delta t / \Delta x \le 0$  then this method is <u>stable</u>;

#### Stable Discretizations: FTBS, FTFS



## The 1<sup>st</sup> Order Godunov Method

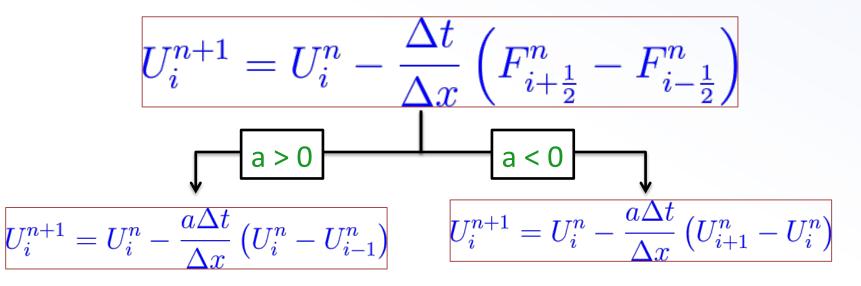
• Summarizing: the stable discretization makes use of the grid point where information is coming from:



• This is also called the first-order Godunov method;

#### **Conservative Form**

• Define the "flux" function  $F_{i+\frac{1}{2}}^n = \frac{a}{2} \left( U_{i+1}^n + U_i^n \right) - \frac{|a|}{2} \left( U_{i+1}^n - U_i^n \right)$ so that Godunov method can be cast in *conservative* form



 The conservative form ensures a correct description of <u>discontinuities</u> in nonlinear systems, ensures global conservation properties and is the main building block in the development of high-order <u>finite volume</u> schemes.  Since the advection speed *a* is a parameter of the equation, ∆x is fixed from the grid, the previous inequality is a <u>stability constraint</u> on the time step for <u>explicit methods</u>

$$\Delta t \le \frac{\Delta x}{|a|}$$

- *∆t* cannot be arbitrarily large but, rather, less than the time taken to travel one grid cell (CFL) condition.
- In the case of nonlinear equations, the speed can vary in the domain and the maximum of *a* should be considered instead.

#### **III. NONLINEAR HYPERBOLIC PDE**

• We turn our attention to the scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

- Where f(u) is, in general, a nonlinear function of u.
- To gain some insights on the role played by nonlinear effects, we start by considering the inviscid Burger's equation:

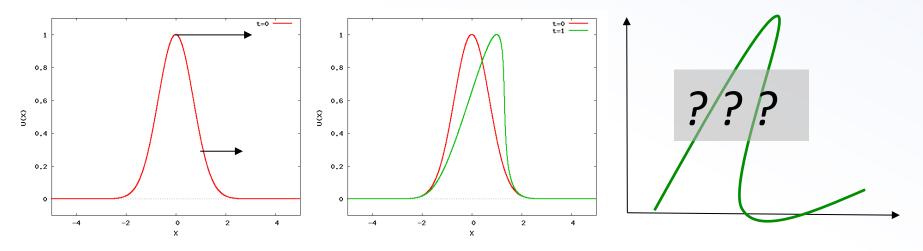
$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{u^2}{2}\right) = 0$$

- We can write Burger's equation also as  $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$
- In this form, Burger's equation resembles the linear advection equation, except that the velocity is no longer constant but it is equal to the solution itself.
- The characteristic curve for this equation is

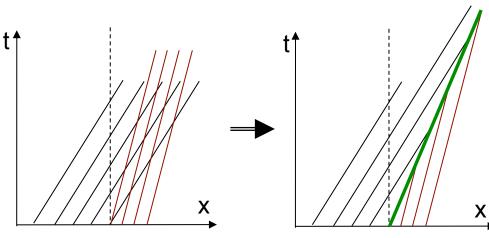
$$\frac{dx}{dt} = u(x,t) \implies \frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt} = 0$$

 → u is constant along the curve dx/dt=u(x,t) → characteristics are again straight lines: values of u associated with some fluid element do not change as that element moves.

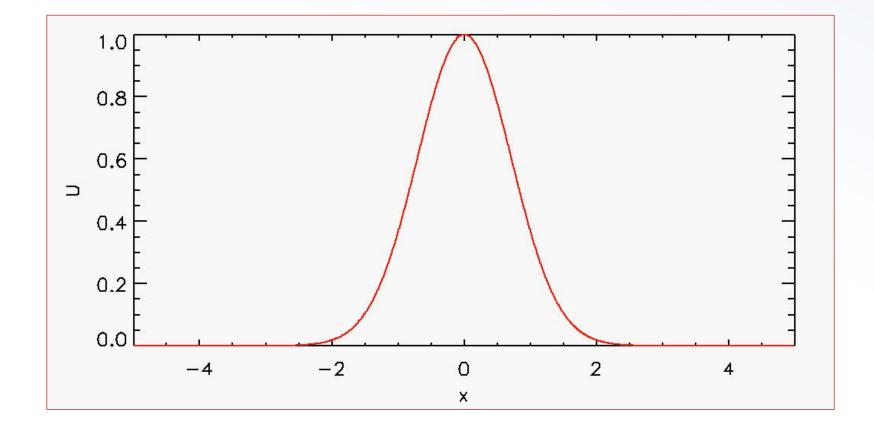
• From  $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$  one can predict that higher values of u will propagate faster than lower values:  $\rightarrow$  wave steepening.



 Correct answer: characteristic will intersect creating a *shock wave*:



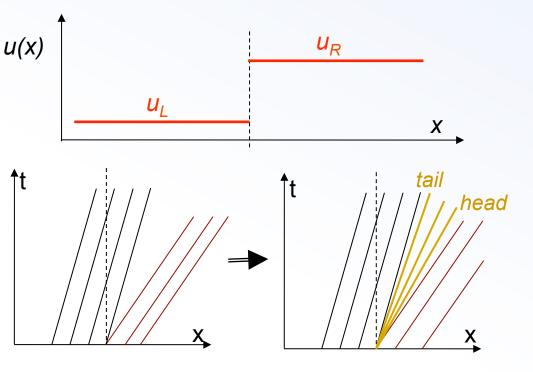
• This is how the solution should look like:



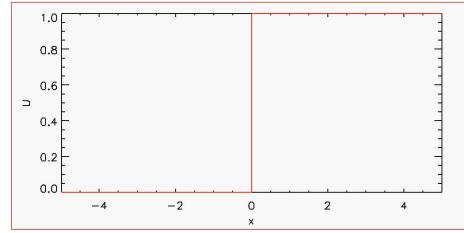
• Such solutions to the PDE are called *weak solutions*.

• In the opposite situation: <sup>4</sup>

 Here characteristic velocities on the left are smaller than those on the right →



 The proper solution is a rarefaction (expansion) wave, a nonlinear self-similar wave that smoothly connects L/R states.

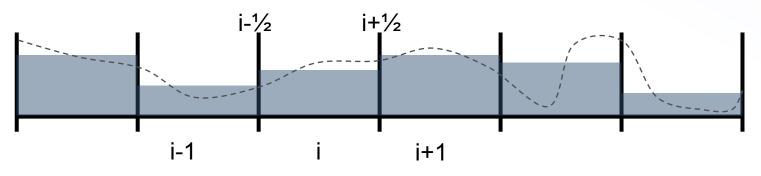


## **IV. FINITE VOLUME METHODS**

• In a finite volume discretization, the unknowns are the spatial averages of the function itself:

$$\langle U \rangle_i^n = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} U(x,t^n) \, dx$$

where  $x_{i-\frac{1}{2}}$  and  $x_{i+\frac{1}{2}}$  denote the location of the cell interfaces.



• The solution to the conservation law involves computing fluxes through the boundary of the control volumes

• The *conservative form* links the *differential* form of the equation and its integral representation:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad \Longrightarrow \quad \int_{t^n}^{t^{n+1}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left(\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x}\right) = 0$$

obtained by integrating the PDE over a time interval  $\Delta t = t^{n+1} - t^n$ and cell size  $\Delta x = x_{i+1/2} - x_{i-1/2}$ 

$$\langle U \rangle_i^{n+1} = \langle U \rangle_i^n - \frac{\Delta t}{\Delta x} \left( \tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n-\frac{1}{2}} \right)$$

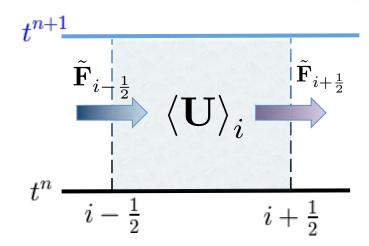
where 
$$\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} F(x_{i+\frac{1}{2}}, t) dt$$

## **Finite Volume Formulation**

$$\langle U \rangle_{i}^{n} = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} U(x,t^{n}) \, dx \qquad \tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{\Delta t} \int_{t^{n}}^{t^{n+1}} F(x_{i+\frac{1}{2}},t) \, dt$$

$$\underline{Orm} \quad \langle U \rangle_{i}^{n+1} = \langle U \rangle_{i}^{n} - \frac{\Delta t}{\Delta x} \left( \tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n-\frac{1}{2}} \right)$$

Integral form

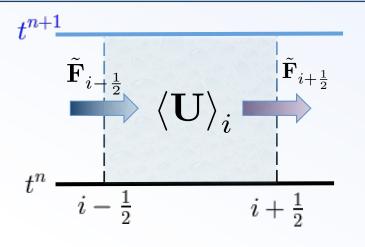


- This is an <u>EXACT</u> evolutionary equation for the spatial averages of U.
- The integral form does not make use of partial derivatives!
- Problem: how do we compute the flux ?

# Flux computation: the Riemann Problem

 Since the solution is known only at t<sup>n</sup>, some kind of approximation is required in order to evaluate the flux through the boundary:

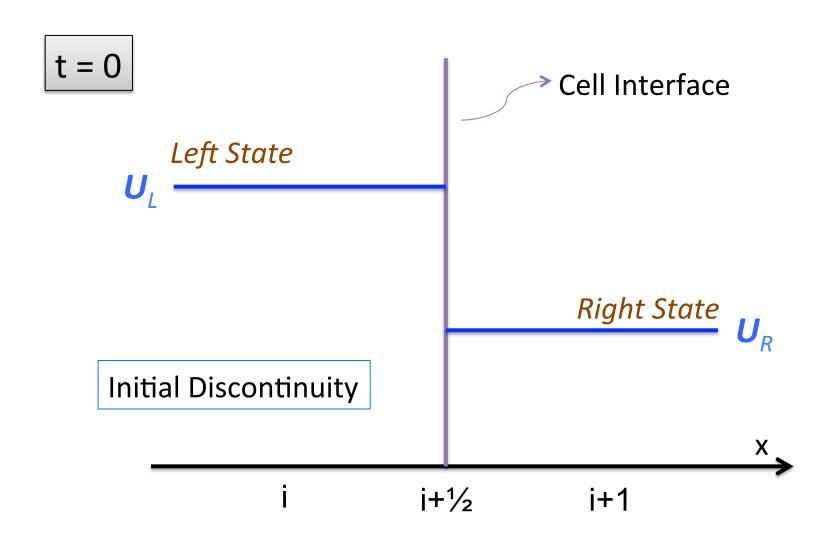
$$\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} F(x_{i+\frac{1}{2}}, t) \, dt$$



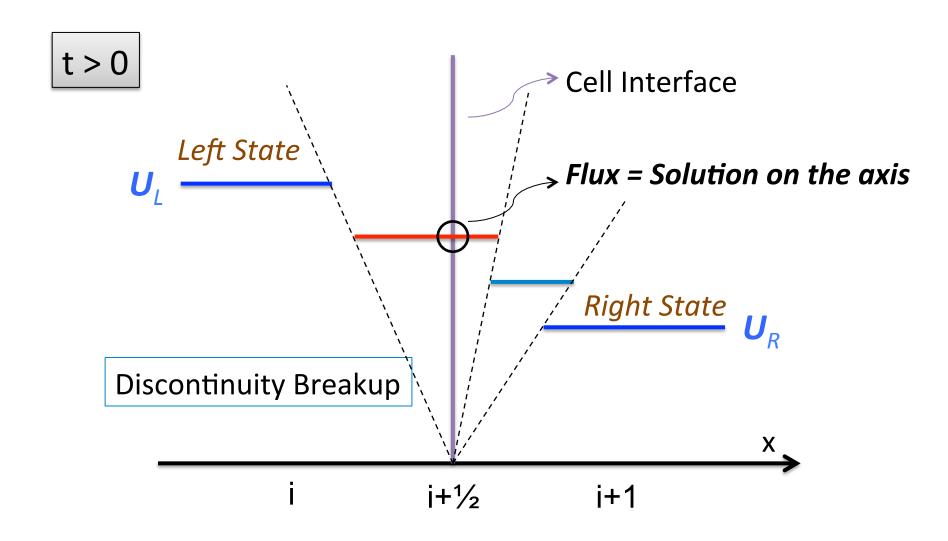
 This achieved by solving the so-called "*Riemann Problem*", i.e., the evolution of an inital discontinuity separating two <u>constant</u> states. The Riemann problem is defined by the initial condition:

$$U(x,0) = \begin{cases} U_L & \text{for } x < x_{i+\frac{1}{2}} \\ U_R & \text{for } x > x_{i+\frac{1}{2}} \end{cases} \implies U(x_{i+\frac{1}{2}}, t > 0) =?$$

#### **The Riemann Problem**

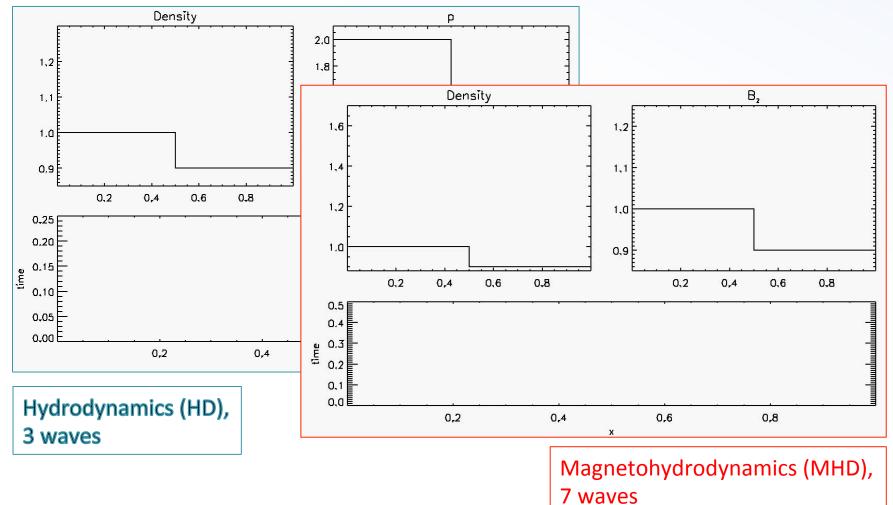


#### The Riemann Problem

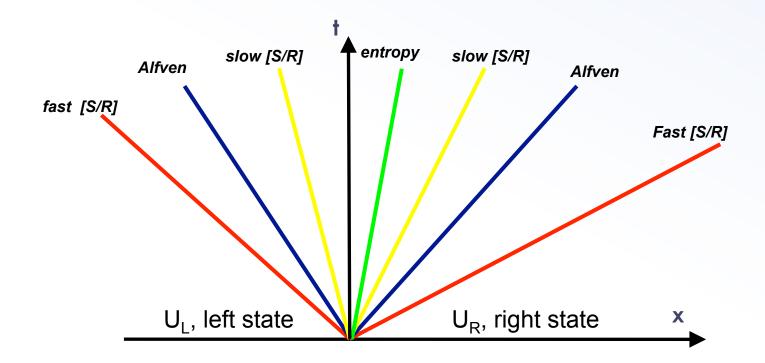


# **The Riemann Problem**

• In CFD, the solution to the Riemann problem depends on the underlying system of conservation laws:



#### Riemann Problem in MHD/Relativistic MHD

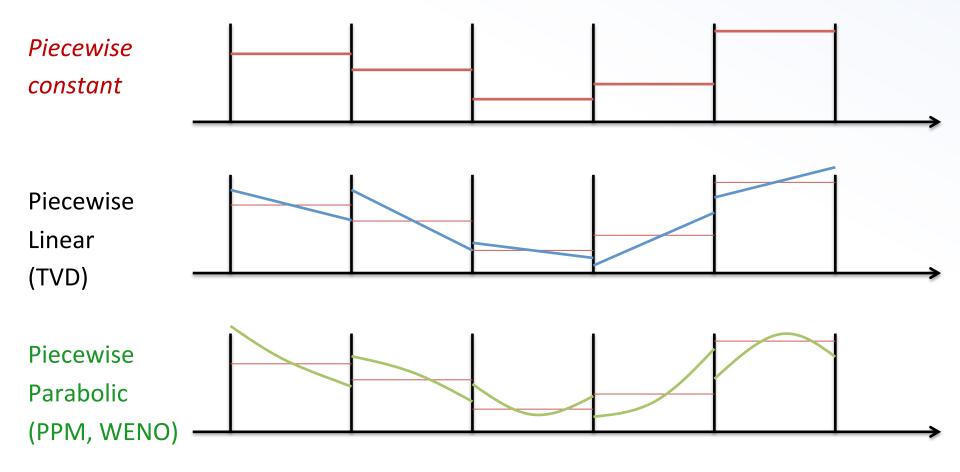


- 7 wave pattern,  $\lambda^{(\kappa)} \left( \boldsymbol{U}_{L}^{(\kappa)} \boldsymbol{U}_{R}^{(\kappa)} \right) = \boldsymbol{F} \left( \boldsymbol{U}_{L}^{(\kappa)} \right) \boldsymbol{F} \left( \boldsymbol{U}_{R}^{(\kappa)} \right)$
- across the contact wave, for  $B_n \neq 0$ , only density has a jump;
- across Alfven waves, [ρ] = [p<sub>gas</sub>]=0 but normal velocity [v<sub>x</sub>]≠ 0
   →magnetic field circularly / elliptically polarized.

- Riemann solvers generalized the concept of "<u>upwind</u>" to nonlinear systems of hyperbolic PDE: the discretization is biased towards the direction of propagation of waves.
- The Riemann problem requires the solution of nonlinear systems of equations.
- Exact solutions are computational expensive !
  - $\rightarrow$  approximate methods preferred:
    - Linearized solvers (Roe-like)
    - *approximate Riemann fan* with fewer waves (more diffusive, HLL, HLLC, HLLD, Lax-Friedrichs);

# Improving spatial accuracy

• High order reconstruction can be carried inside each cell by suitable oscillation-free polynomial interpolation:



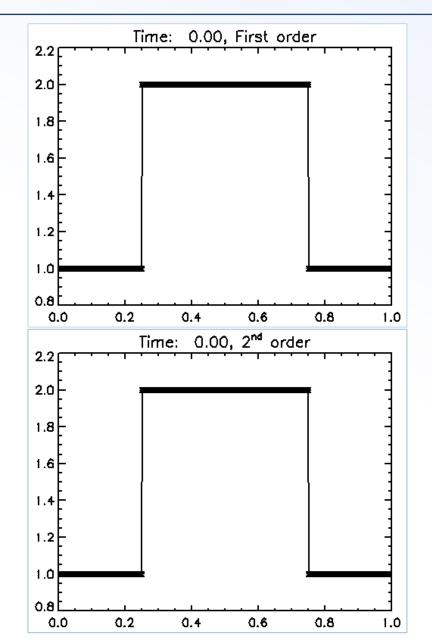
#### 1<sup>st</sup> and 2<sup>nd</sup> Order Reconstruction

• 1<sup>st</sup> First-order reconstruction:

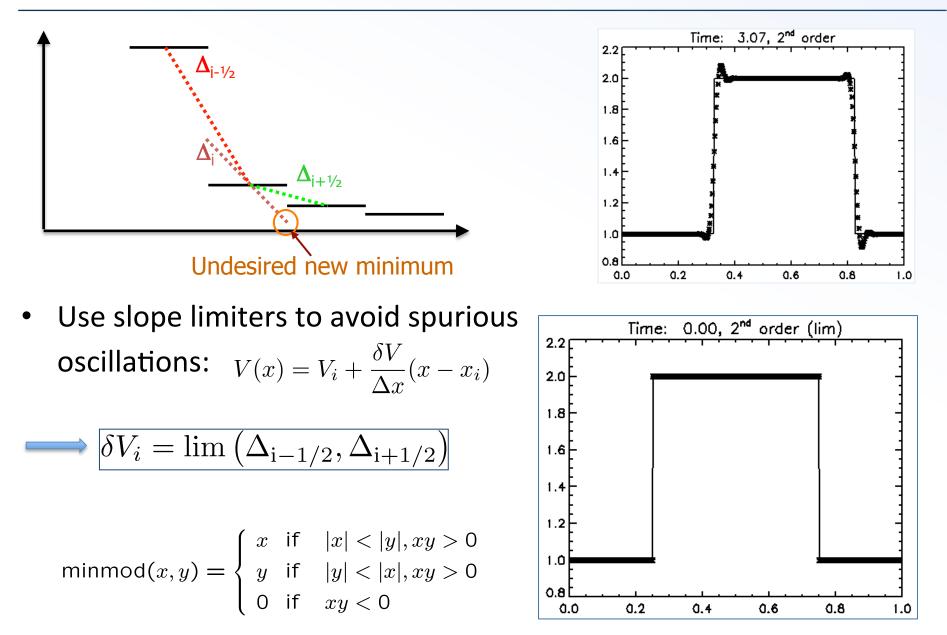
 $V(x) = V_i$ 

• For 2<sup>nd</sup>-order we use linear reconstrution:

$$V(x) = V_i + \frac{\delta V}{\Delta x}(x - x_i)$$



### **Preventing Oscillations**

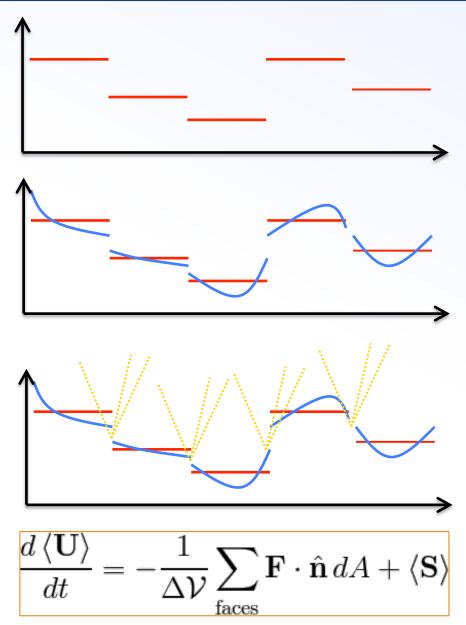


### **Reconstruct-Solve-Update**

- Start from volume-averages  $\langle {f U} 
  angle_i^n$
- Reconstruct interface values from zone averages using a high-order non-oscillatory polynomial:

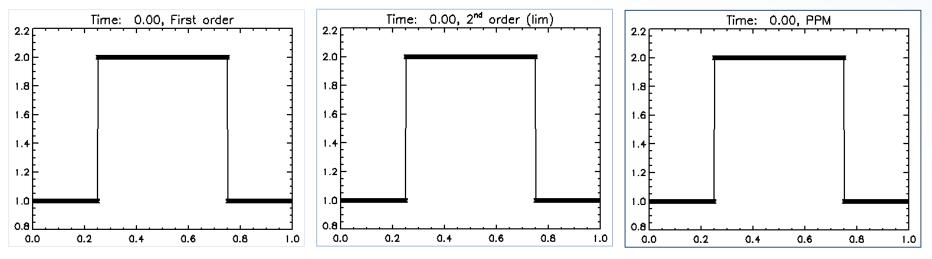
 $\begin{cases} \mathbf{U}_{i+\frac{1}{2}}^{L} = \lim_{x \to x_{i+\frac{1}{2}}^{-}} \mathbf{U}_{i}(x) ,\\ \mathbf{U}_{i+\frac{1}{2}}^{R} = \lim_{x \to x_{i+\frac{1}{2}}^{+}} \mathbf{U}_{i+1}(x) , \end{cases}$ 

- Solve Riemann problems between adjacent, discontinuous states.
   → Compute interface flux.
- Update conserved variables with time stepping algorithm (e.g. RK2):



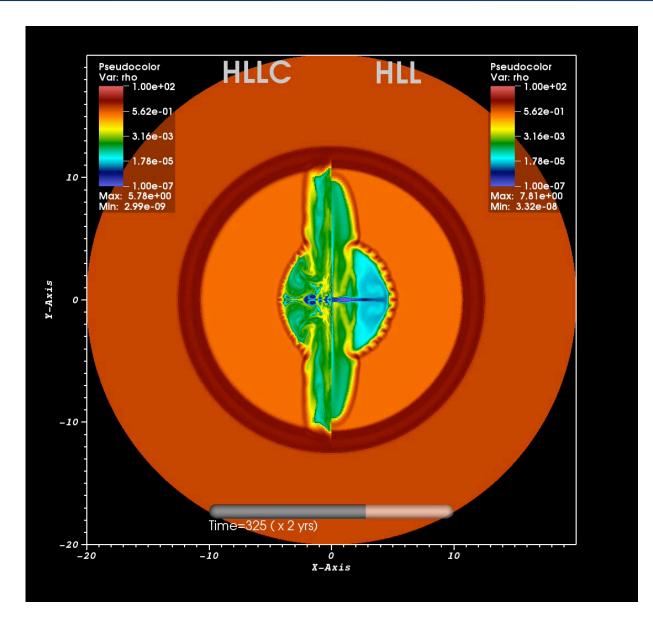
# Numerical Diffusion

- Generally, the amount of numerical diffusion is controlled by the underlying grid resolution / numerical scheme:
  - spatial reconstruction
  - Riemann solver accuracy
  - (marginally) time stepping



- PROS: numerical diffusion has a stabilizing effect.
- CONS: suppress small scale effect, may prevent growth of instabilities

#### A 2D Example: Axisymmetric PWN



#### Popular MHD Open Source codes

	AMR	Language	Relat. MHD	Main developer
Athena	*	С	~	J. Stone et al.
FLASH	~	Fortran (?)	*	P. Tzeferacos et al.
PLUTO	~	C, C++	~	A. Mignone et al.
Ramses	~	Fortran90	*	R. Teyssier et al.
Pencil	?	Fortran90	*	A. Brandenburg
VAC	~	Fortran90+Perl	~	Van Der Holst / Meliani /Porth

#### V. BEYOND IDEAL MHD

### **Beyond Ideal MHD**

- The range of validity of MHD can be extended by several means, at the cost of introducing additional terms and more complex algorithms.
- One will then have to deal with *different time scales*.
- Example are:
  - *Dissipative effects* (viscosity, Ohmic dissipation, thermal conduction, etc...)
     → mixed hyperbolic / parabolic PDE.
  - Extended MHD including generalized Ohm's law (Hall-MHD, electron pressure) → dispersive waves, non-homogenous PDE with stiff sources (RMHD);
  - Fluid-particles *hybrid* algorithms.

- Parabolic (diffusion) term describes transfer of momentum or energy due to microscopical processes without requiring bulk motion.
- Examples: viscosity, magnetic resistivity, thermal conduction.

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) &= 0 \\ \frac{\partial (\rho \boldsymbol{v})}{\partial t} + \nabla \cdot \left[ \rho \boldsymbol{v} \boldsymbol{v}^T - \boldsymbol{B} \boldsymbol{B}^T \right] + \nabla p_t &= \nabla \cdot \boldsymbol{\tau} + \rho \boldsymbol{g} \\ \frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \left[ (\mathcal{E} + p_t) \, \boldsymbol{v} - (\boldsymbol{v} \cdot \boldsymbol{B}) \, \boldsymbol{B} \right] &= \nabla \cdot \boldsymbol{\Pi}_{\mathcal{E}} - \boldsymbol{\Lambda} + \rho \boldsymbol{v} \cdot \boldsymbol{g} \\ \frac{\partial \boldsymbol{B}}{\partial t} - \nabla \times (\boldsymbol{v} \times \boldsymbol{B}) &= -\nabla \times (\eta \boldsymbol{J}) \\ \frac{\partial (\rho X_{\alpha})}{\partial t} + \nabla \cdot (\rho X_{\alpha} \boldsymbol{v}) &= \rho S_{\alpha} \end{aligned}$$

 No upwinding is required since parabolic problems have infinite propagation speed → central differences are OK!

### **Explicit Scheme for Parabolic PDE**

- However, explicit schemes subject to restrictive constraint:
- In 1-D with constant D:

$$\frac{\partial U}{\partial t} = D \frac{\partial^2 U}{\partial x^2}$$

- Using FTCS:  $U_i^{n+1} = U_i^n + C(U_{i-1}^n 2U_i^n + U_{i+1}^n)$
- Where  $C = D\Delta t / \Delta x^2$  is the (parabolic) CFL number
- Stability demands  $C \leq \frac{1}{2} \rightarrow \Delta t \leq \Delta x^2 / (2D)$
- This is quite restrictive !

### **Implicit Schemes for Parabolic PDE**

• Using a backward in time, centered in space (BTCS):

 $U_i^{n+1} = U_i^n + C(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1})$ 

has no stability limit (*unconditionally stable !*)

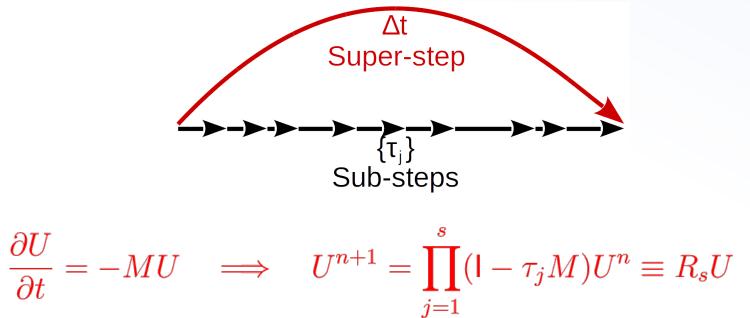
• However, it leads to an implicit (linear) system:

 $\mathsf{A}\{U\}^{n+1} = \{U\}^n, \qquad \mathsf{A} \in \mathbb{R}^{N_x \times N_x}$ 

- This is a global operation and thus not can not be efficiently carried out on parallel domains.
- Alternative  $\rightarrow$  Accelerated explicit methods  $\rightarrow$

# **Accelerated Explicit Methods**

 Divide each time step Δt in s sub-steps based on a polynomial sequence and require stability at the end of a cycle of s substeps:



- In practice we require the super-step to be as large as possible, exploiting properties of orthogonal polynomial, <u>Chebyshev</u> (Super Time Stepping [STS]) or <u>Legendre</u> (Runge-Kutta Legendre [RKL]).
- The scheme is still explicit !

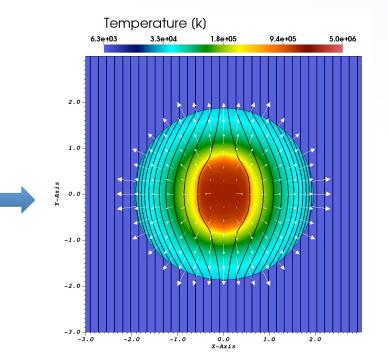
- RKL methods show better stability properties and are preferred over STS.
- Choosing s sub-steps we can cover a time step equal to

$$\Delta t \leq \Delta t_{expl} rac{s^2+s-2}{4}$$

where  $\Delta t_{expl}$  is the standard explicit method time step.

- The method is easily parallelizable.
- Scaling on 2D blast wave:

Algorithm	N <sub>x</sub>	Execution Time [s]
Explicit	192	1 <i>m</i> : 13 <i>s</i>
RKL	192	28 <i>s</i>
Explicit	384	18 <i>m</i> : 32 <i>s</i>
RKL	384	5 <i>m</i> : 19 <i>s</i>
Explicit	768	4 <i>h</i> : 21 <i>m</i> : 15 <i>s</i>
RKL	768	49 <i>m</i> : 17 <i>s</i>
Explicit	1536	3d : 5h : 13m : 10s
RKL	1536	10 <i>h</i> : 4 <i>m</i> : 55 <i>s</i>



#### THE END