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Time-stepping methods (continued) and numerical derivatives

(Pencil Code School, Geneva/CERN, 21st of September 2025)

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Overview:

* Summary on common time-stepping methods

* “Creative” methods for time stepping

* Numerical derivatives

* Numerical curiosities due to precision

* Numerical curiosities from the initial condition

* Numerical curiosities from “switching on” the simulation

Time integration methods

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* may have infinitely growing error

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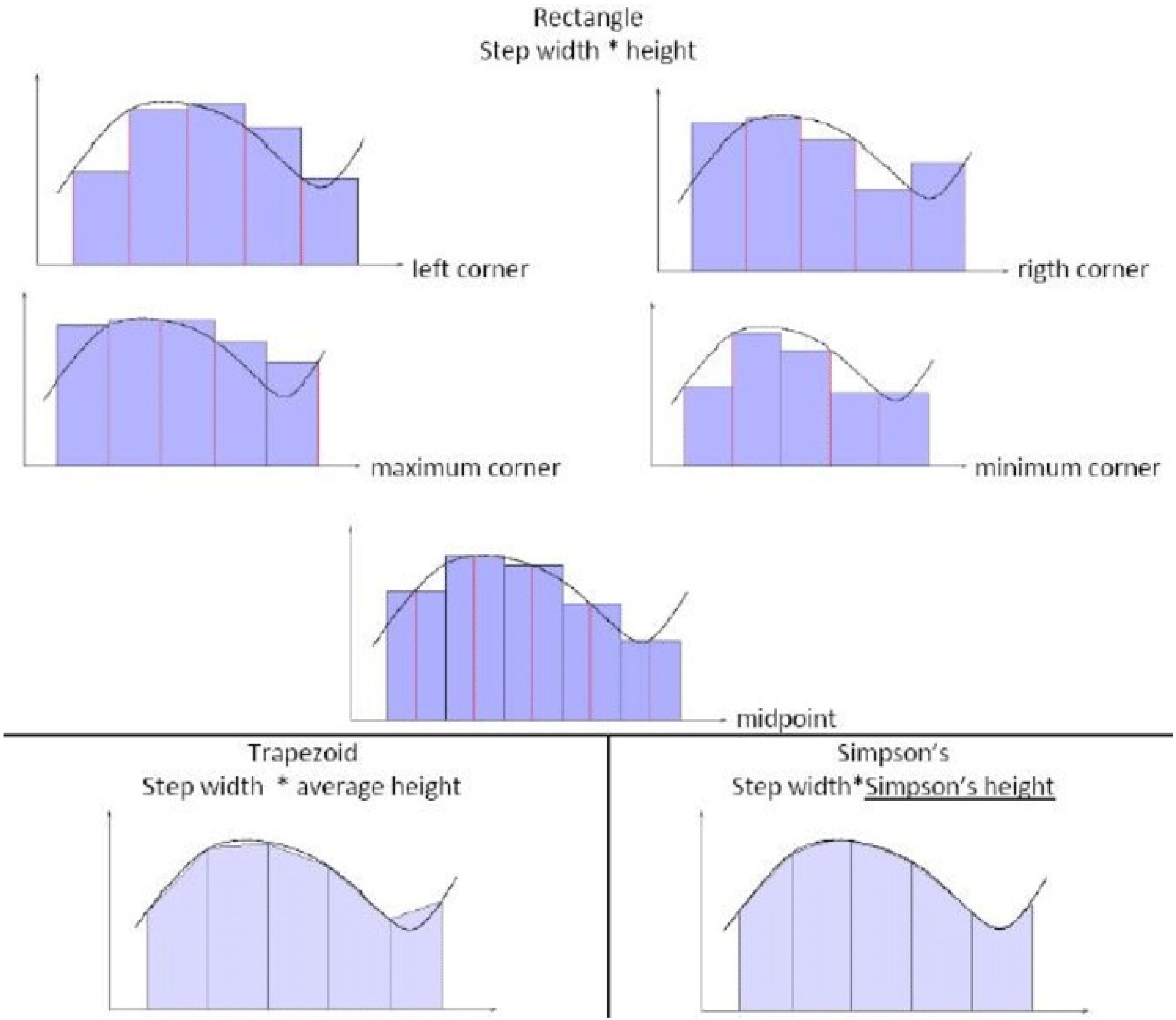
* substeps require additional function evaluations and derivatives (=> costs)

Time integration methods



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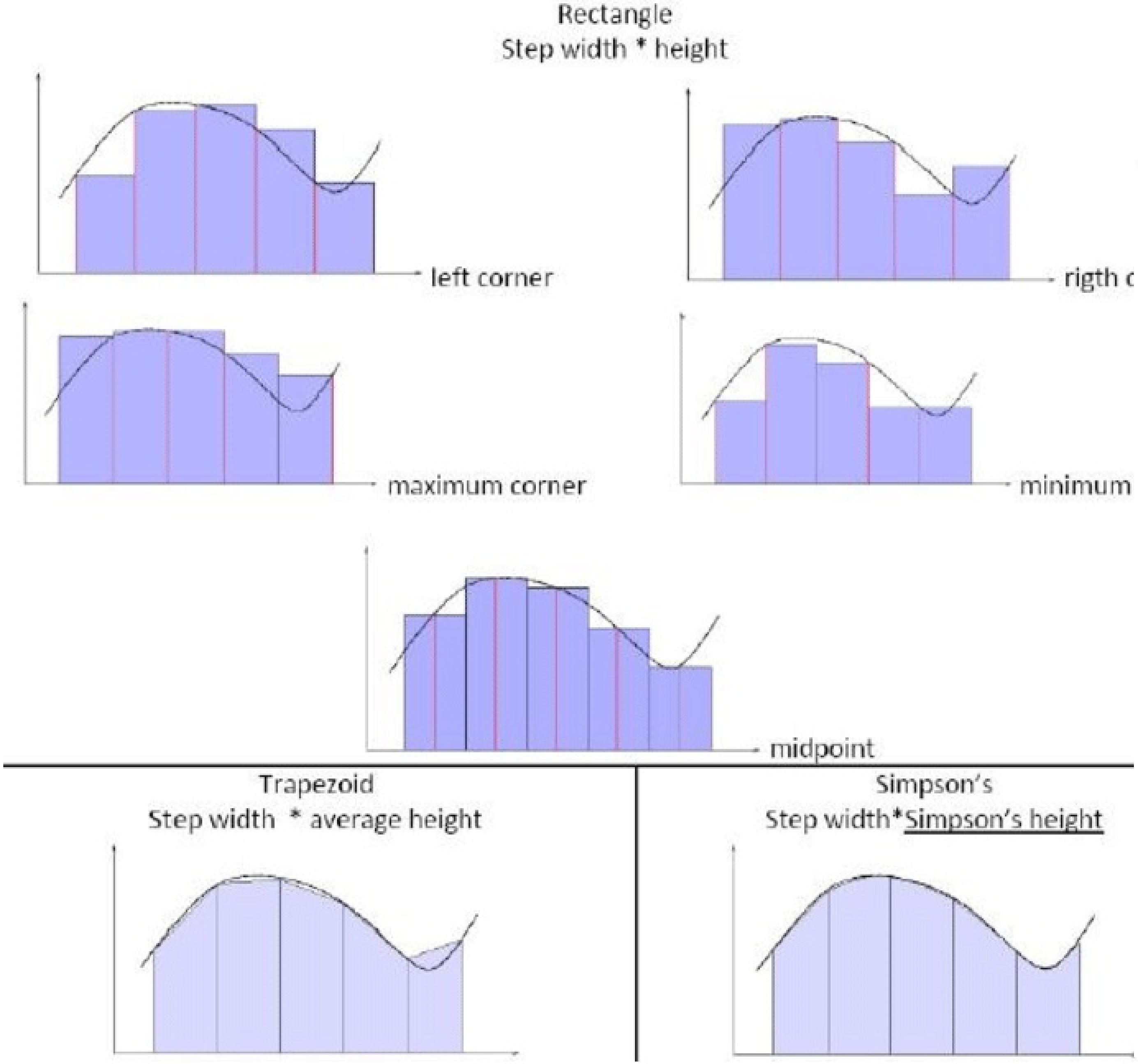
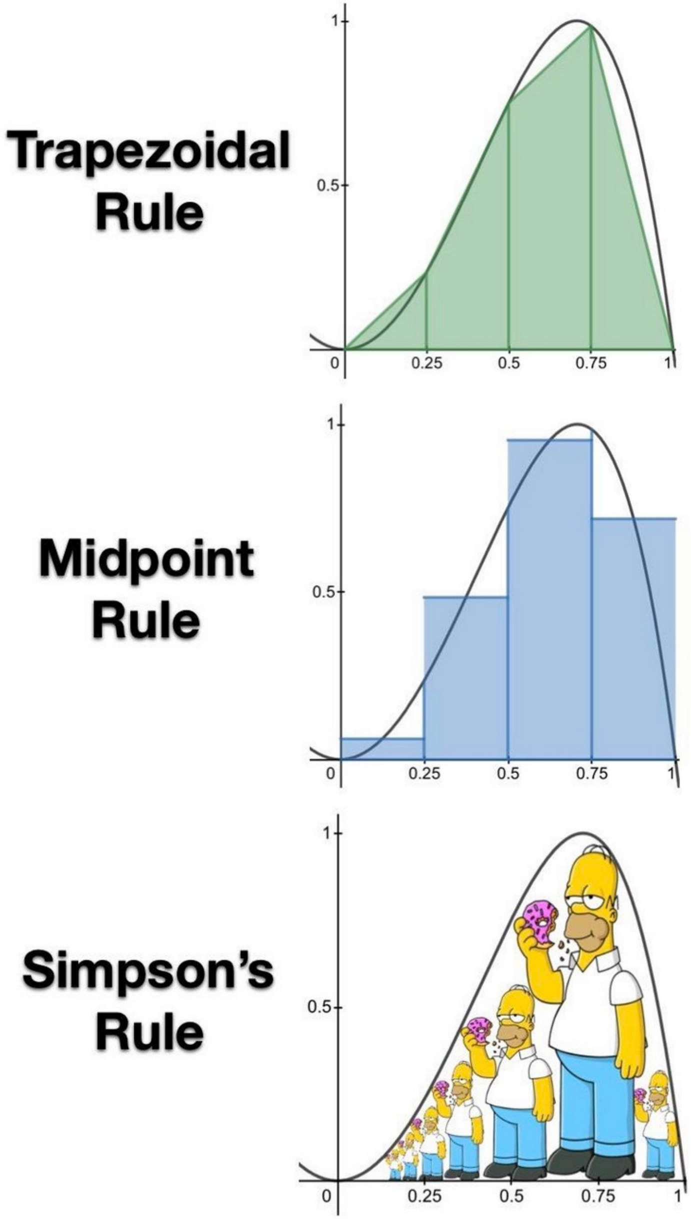




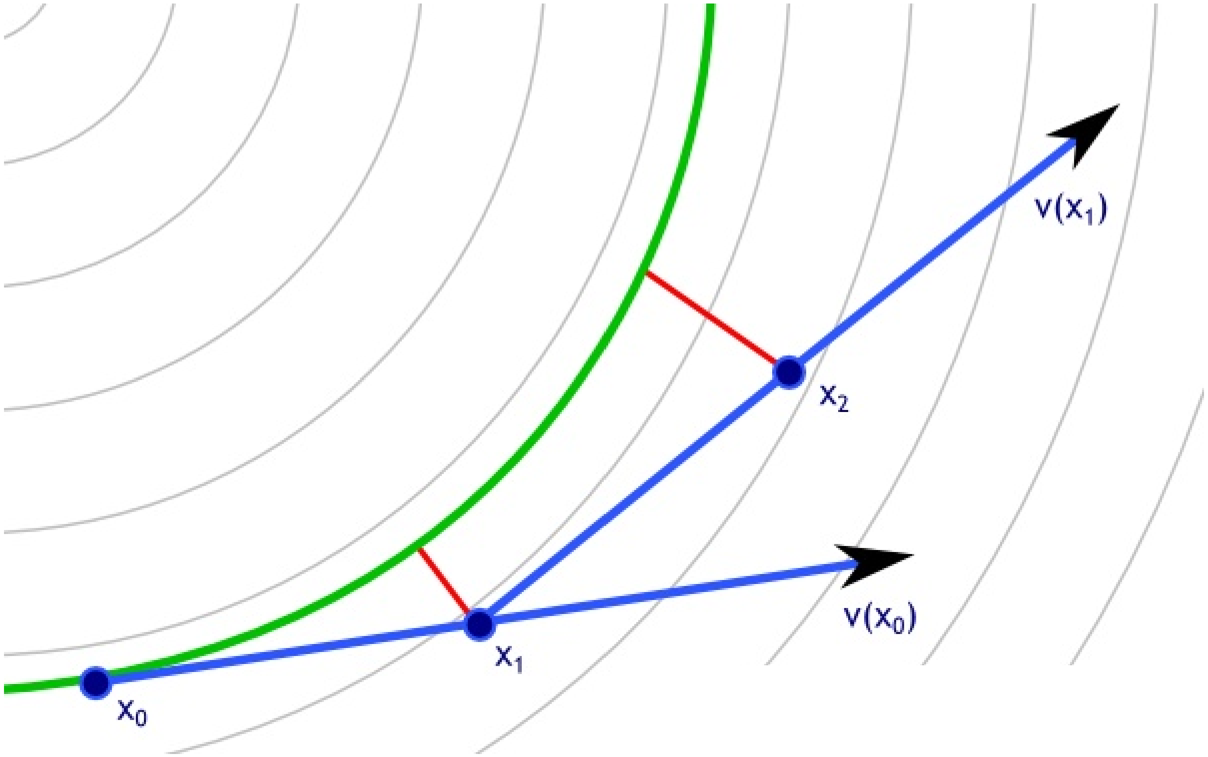
Euler method

Euler method

1) start from x_0
2) calculate derivatives (tangential)

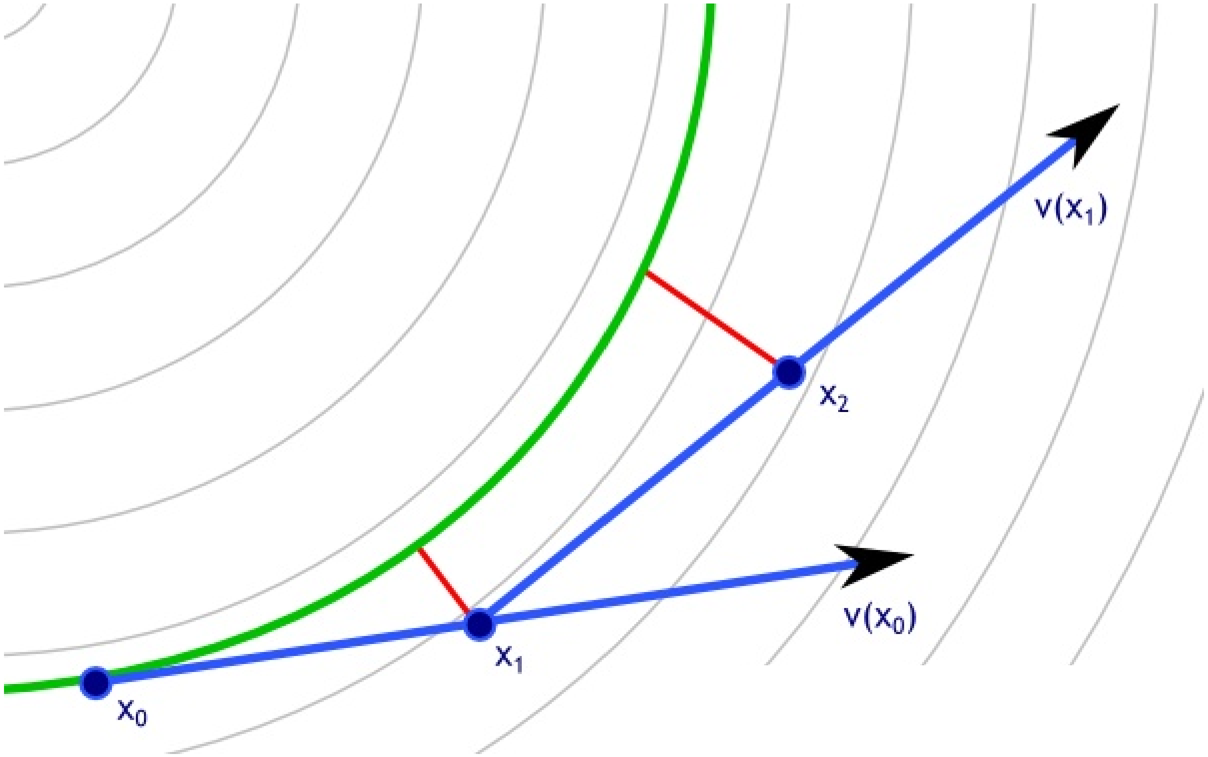
gray: true field

green: exact solution



Euler method

1) start from x_0
2) calculate derivatives (tangential)
3) iterate to x_1 with dt=0.5



green: exact solution

blue: tangential derivative

red: deviation

$$x_{n+1} = x_n + dt \cdot v(x_n) + O(dt^2)$$

x_n : current position

x_{n+1} : next position

dt : time step

$v(x_n)$: vector field at position x_n

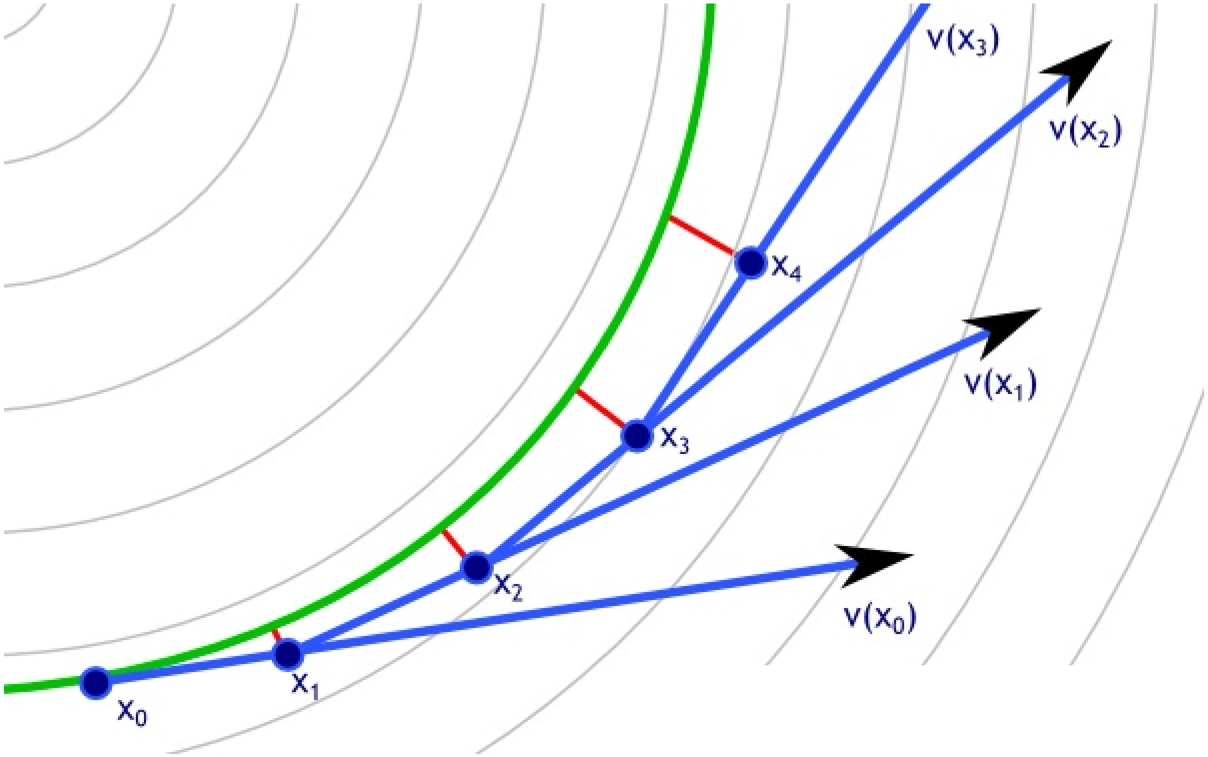
$O(dt^2)$: error

=> error grows infinitely…

=> make dt smaller?

Euler method

1) start from x_0
2) calculate derivatives (tangential)
3) iterate to x_1 with dt=**0.25**



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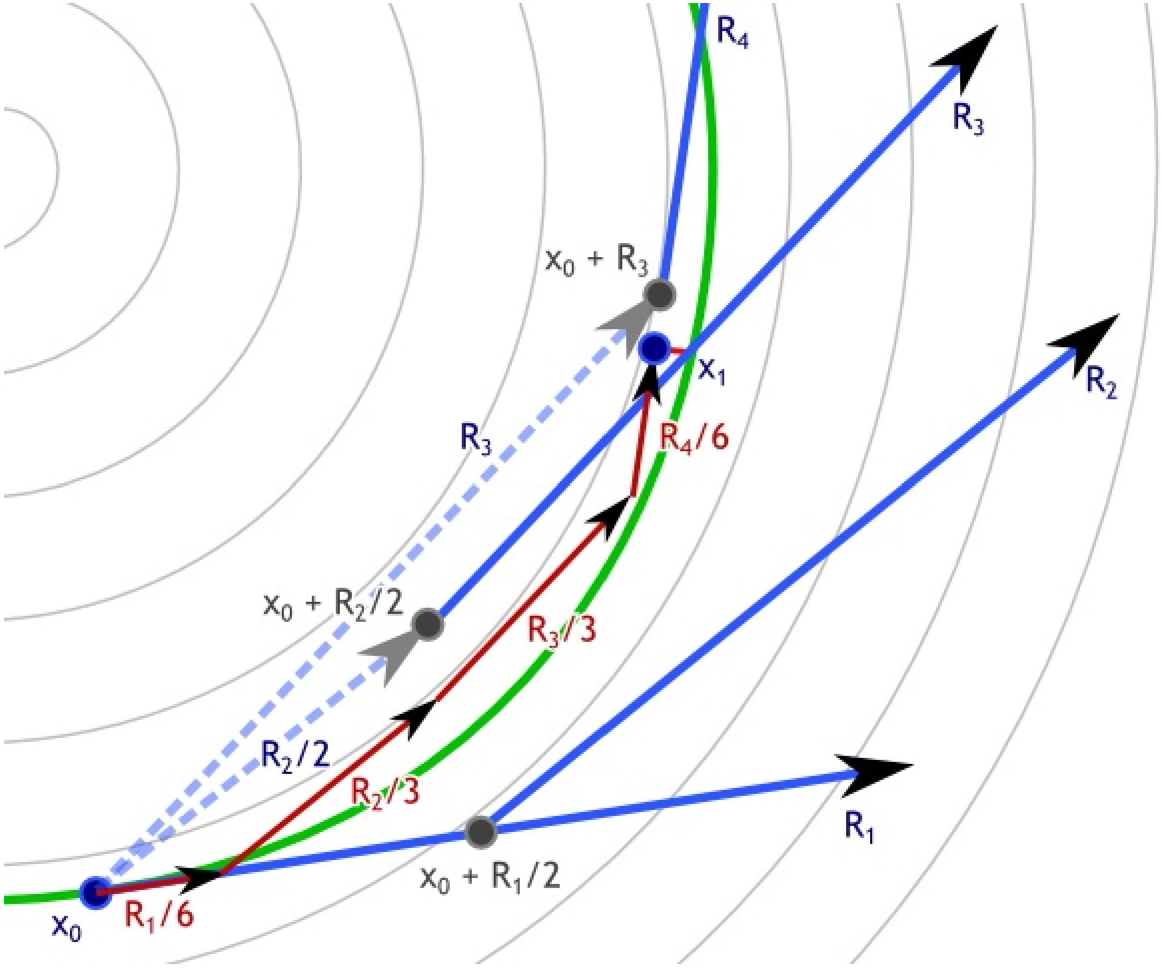
=> accuracy can be improved by making dt smaller

=> but error still grows...

Runge-Kutta method (4th order)

1) start from x_0
2) calculate derivatives (tangential)
3) iterate substeps and recalculate derivatives (tangential)
4) reach x_1 with substeps

blue: tangential derivative
red: deviation



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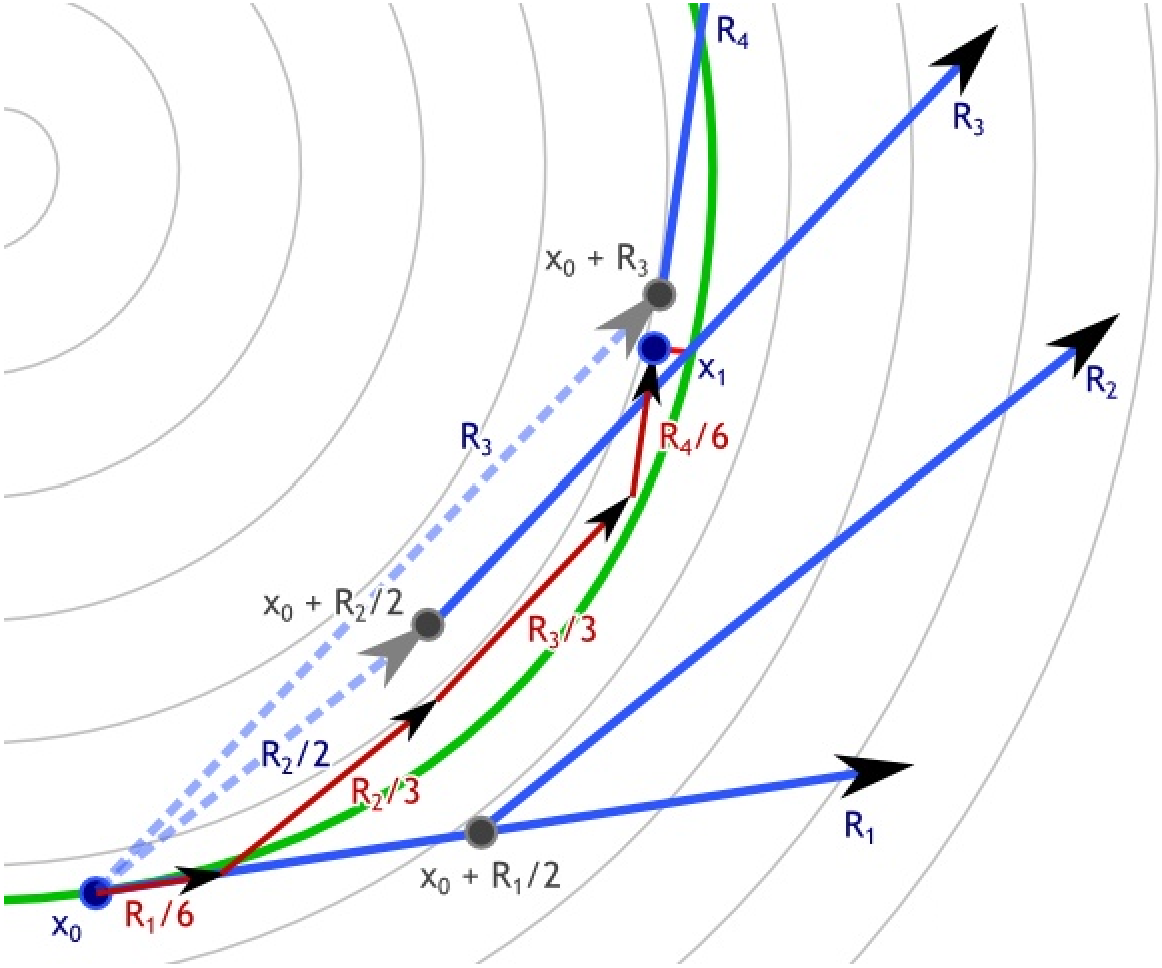

blue: tangential derivative

red: deviation

=> much better accuracy!

=> larger computational cost

Runge-Kutta method (4th order)

RK4 scheme:

$$k_1 = dt \cdot v(x_n)$$

$$k_2 = dt \cdot v(x_n + \frac{k_1}{2})$$

$$k_3 = dt \cdot v(x_n + \frac{k_2}{2})$$

$$k_4 = dt \cdot v(x_n + k_3)$$

$$x_{n+1} = x_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(dt^5)$$

x_n : current position

x_{n+1} : next position

dt : time step

$v(x)$: vector field at position x

$O(dt^5)$: error

“Creative” time-stepping methods

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- Stiff differential equations?

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Small timestep only for fastest dynamics (**timestep_subcycle** with **corona**).

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more timesteps needed & finally not such a big saving of computing time.

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=> Speed up and accuracy granted only in 1D.

“Creative” time-stepping methods

Split Runge-Kutte time step into two halves (**timestep_strang**).

Idea: ...?

=> effects?

“Creative” time-stepping methods

- Split Runge-Kutte time step into two halves (**timestep_strang**).

Idea: ...?

=> effects?

- Algorithms for stiff PDEs (**timestep_stiff** from Numerical Recipies).

Idea: ...?

=> effects?

Numerical derivatives (6th order)

Numerical derivatives (6^{th} order)

Pencil Code manual:

H Numerical methods

H.1 Sixth-order spatial derivatives

Spectral methods are commonly used in almost all studies of ordinary (usually incompressible) turbulence. The use of this method is justified mainly by the high numerical accuracy of spectral schemes. Alternatively, one may use high order finite differences that are faster to compute and that can possess almost spectral accuracy. Nordlund & Stein [32] and Brandenburg et al. [16] use high order finite difference methods, for example fourth and sixth order compact schemes [28].[19]

The sixth order first and second derivative schemes are given by

$$f_i' = (-f_{i-3} + 9f_{i-2} - 45f_{i-1} + 45f_{i+1} - 9f_{i+2} + f_{i+3})/(60\delta x), \tag{235}$$

$$f_i'' = (2f_{i-3} - 27f_{i-2} + 270f_{i-1} - 490f_i + 270f_{i+1} - 27f_{i+2} + 2f_{i+3})/(180\delta x^2), \tag{236}$$

Numerical derivatives (6^{th} order)

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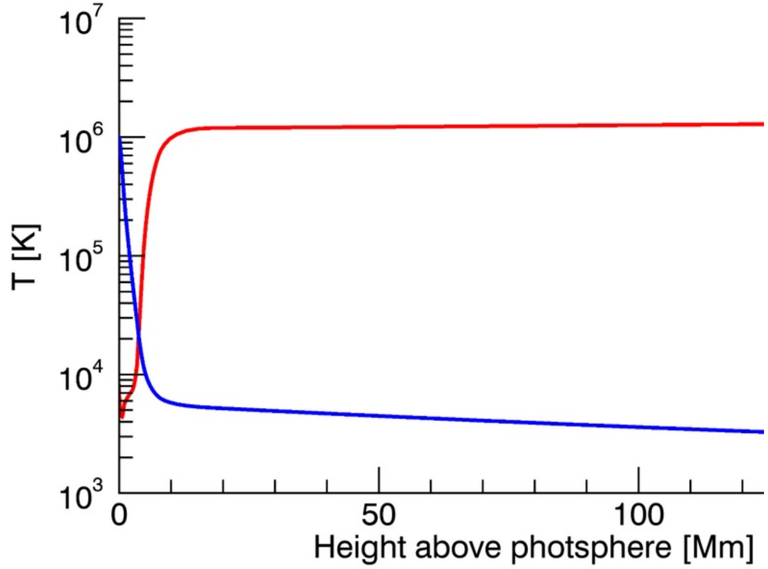
=> Coefficients can be obtained analytically.

Resolving steep gradients in the solar corona

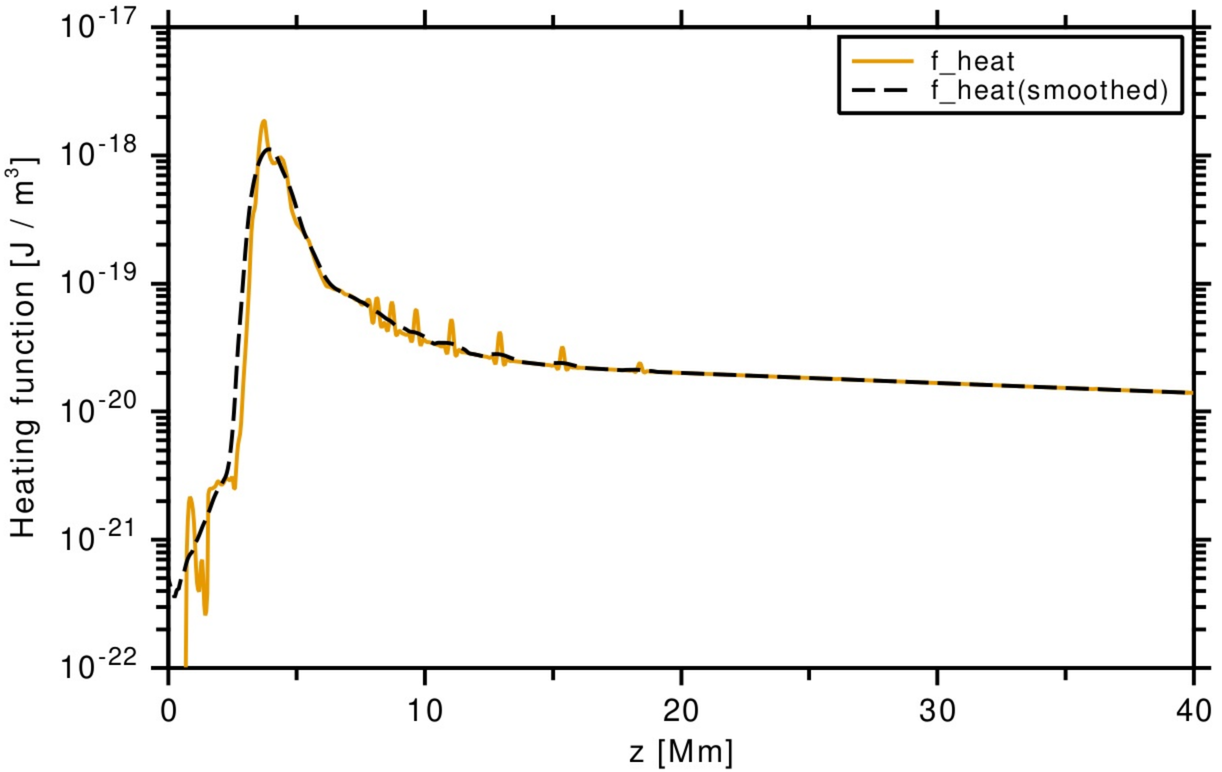
(Vartika Pandey)

Coronal heating in 1D MHD models:

- Initial condition:

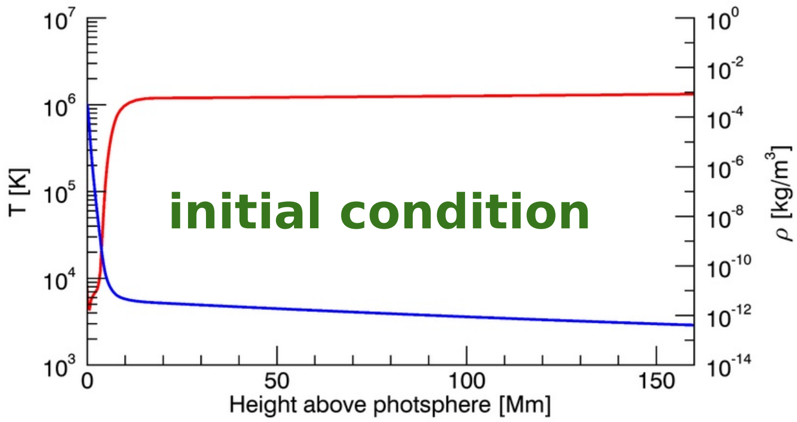


=> After **one** iteration:

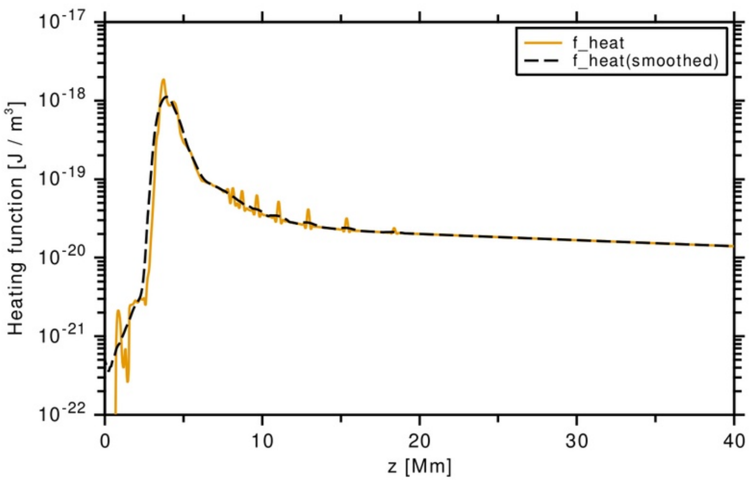


(Pandey & Bourdin, 2025)

Numerical stability analysis:



+ heating



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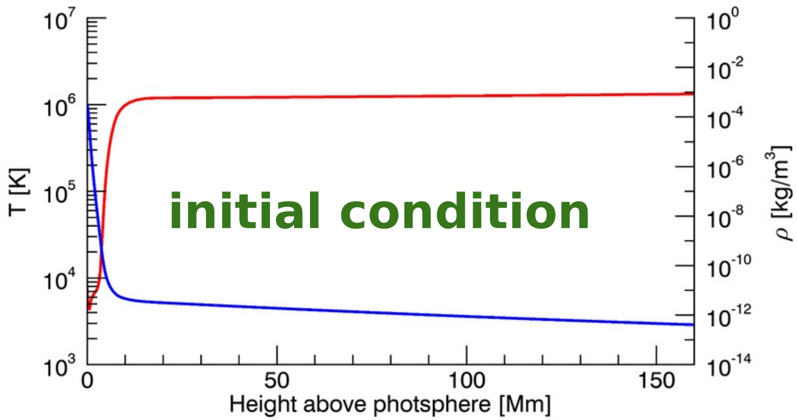

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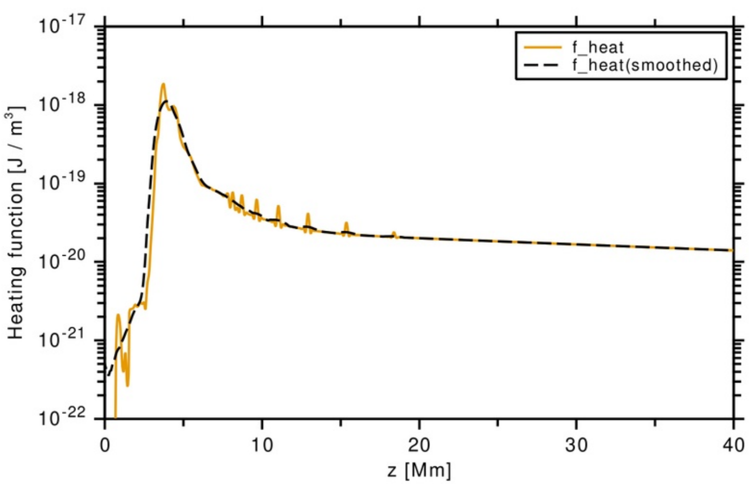

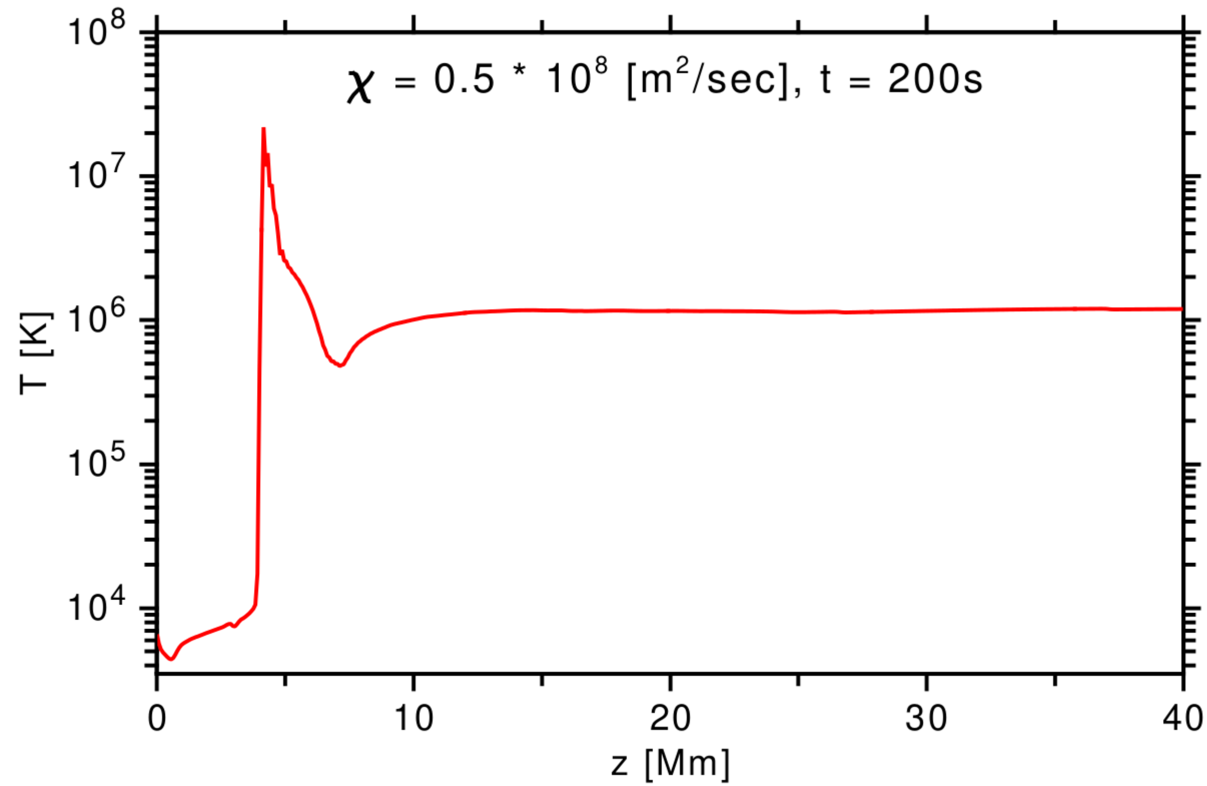

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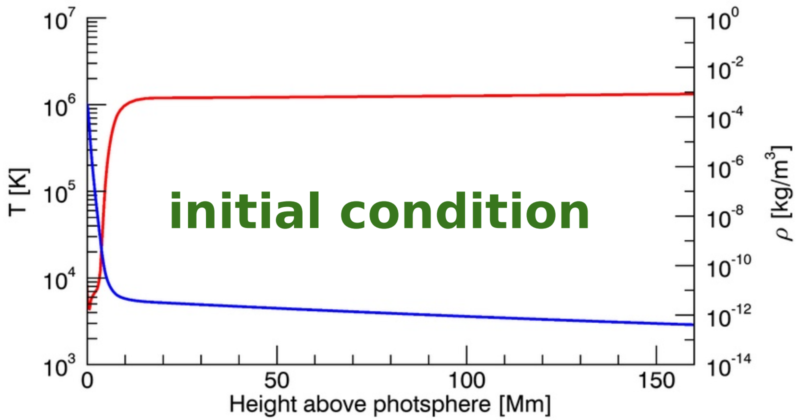
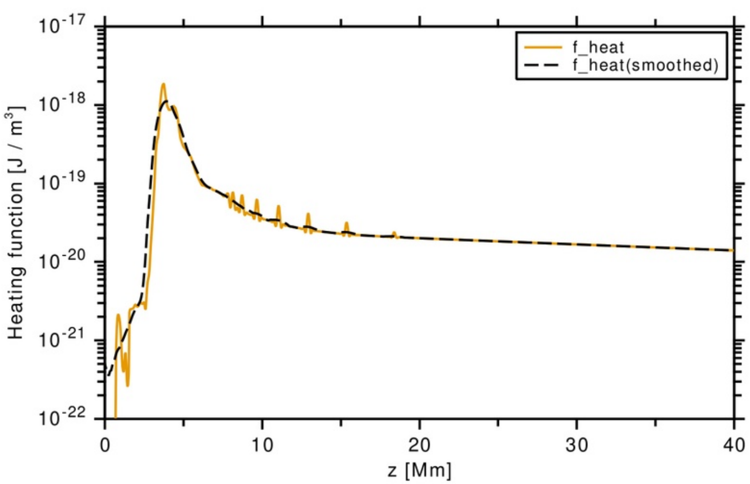
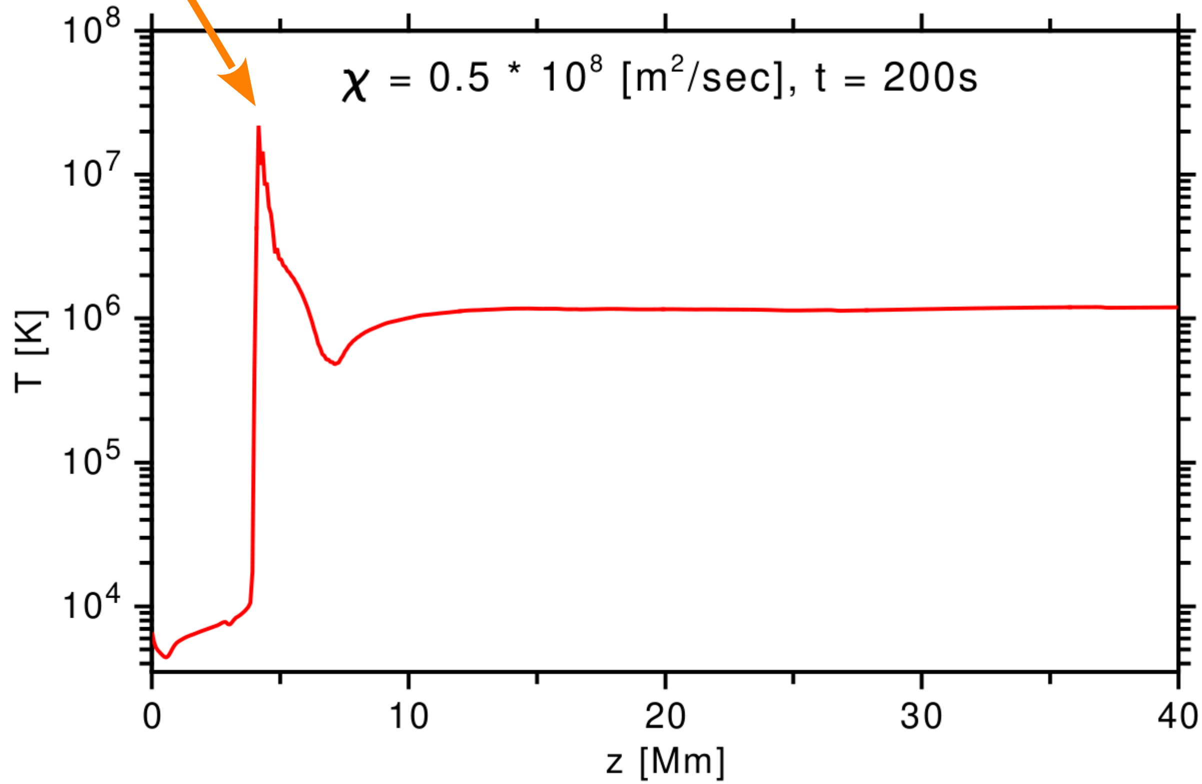


- ? -

+ heating =>



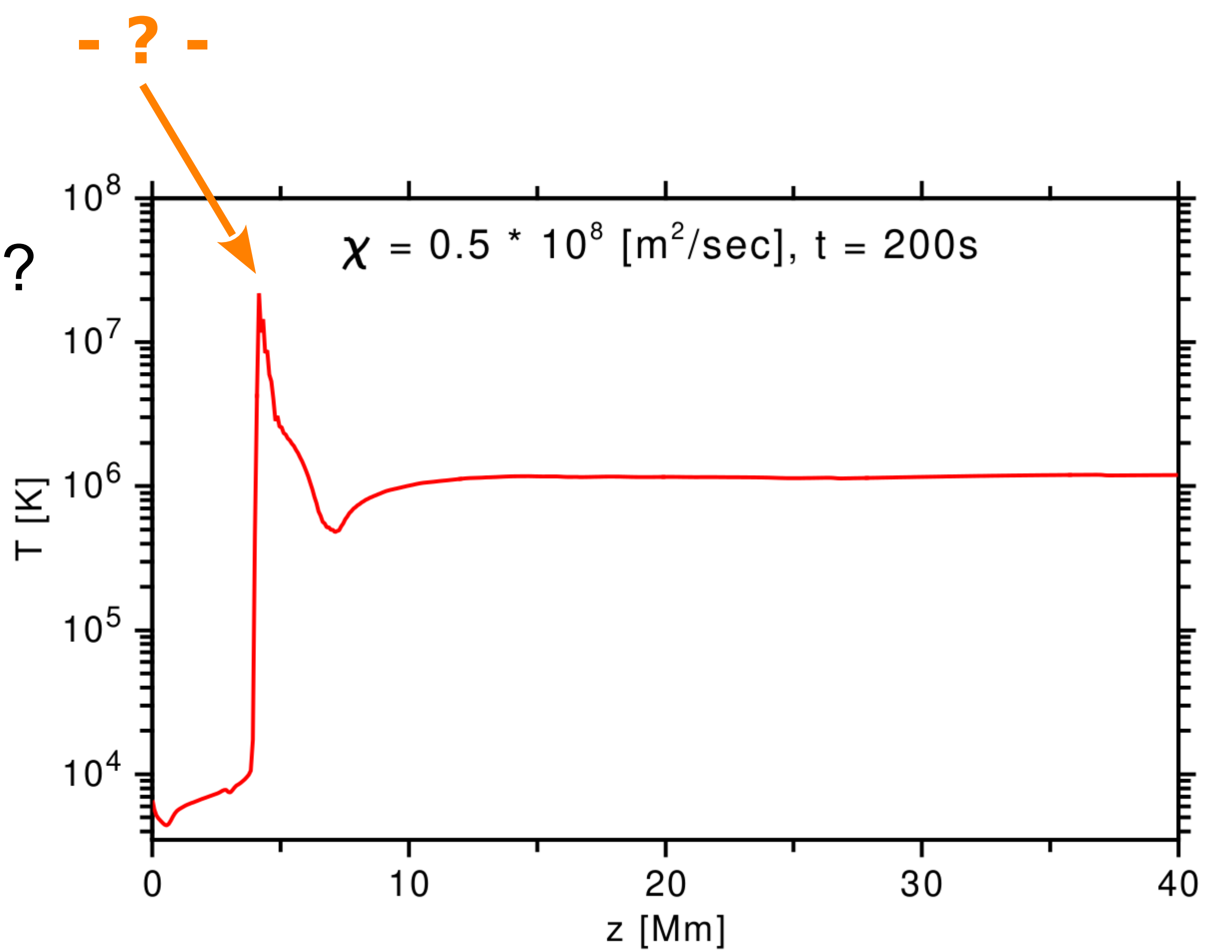


(Pandey & Bourdin, 2025)

Numerical stability analysis:

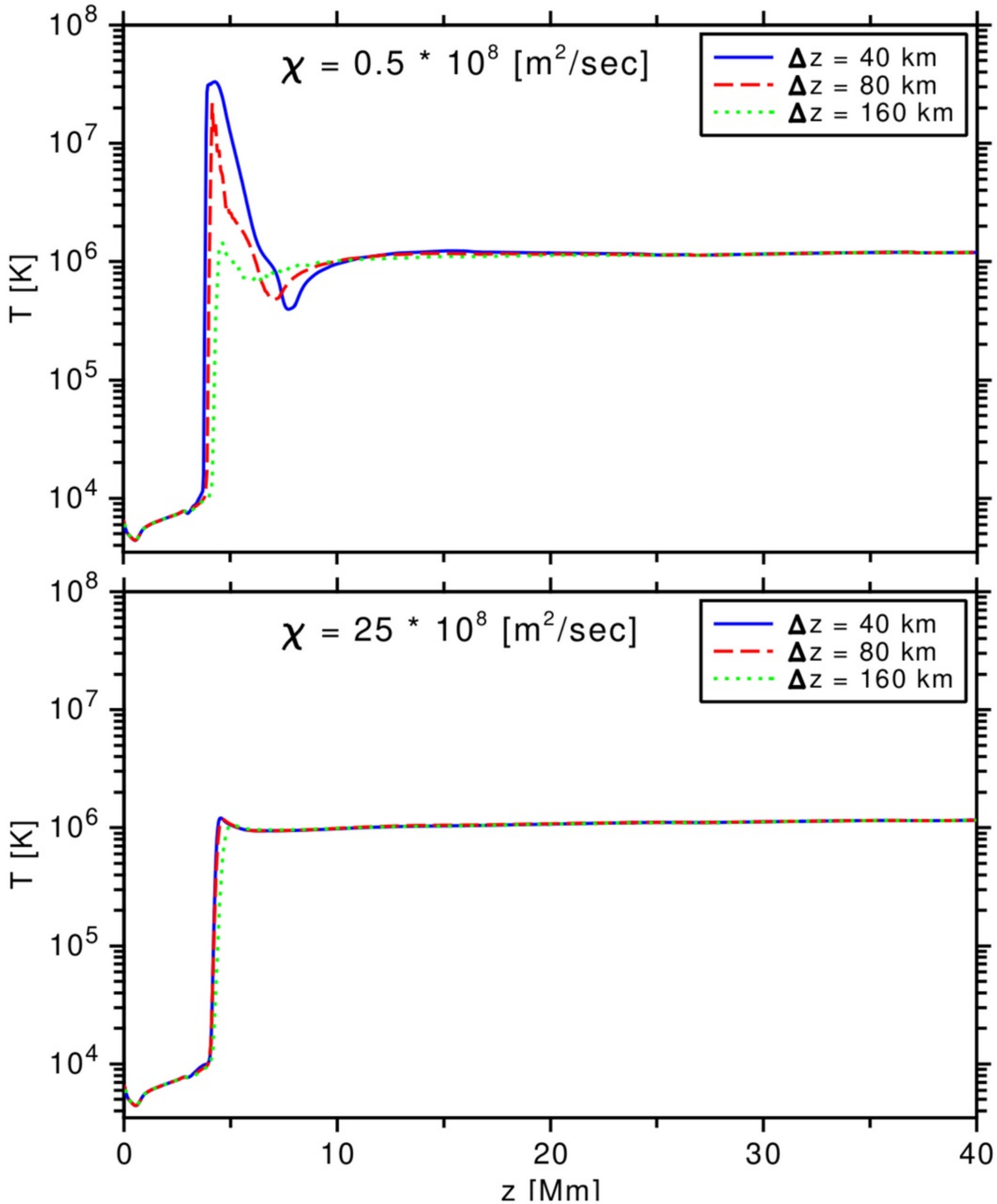
<u>Possible problems:</u>

1) too coarse grid?
2) insufficient diffusion?
3) absence of magnetic field?



(Pandey & Bourdin, 2025)

Effects due to the grid resolution and heat conduction:



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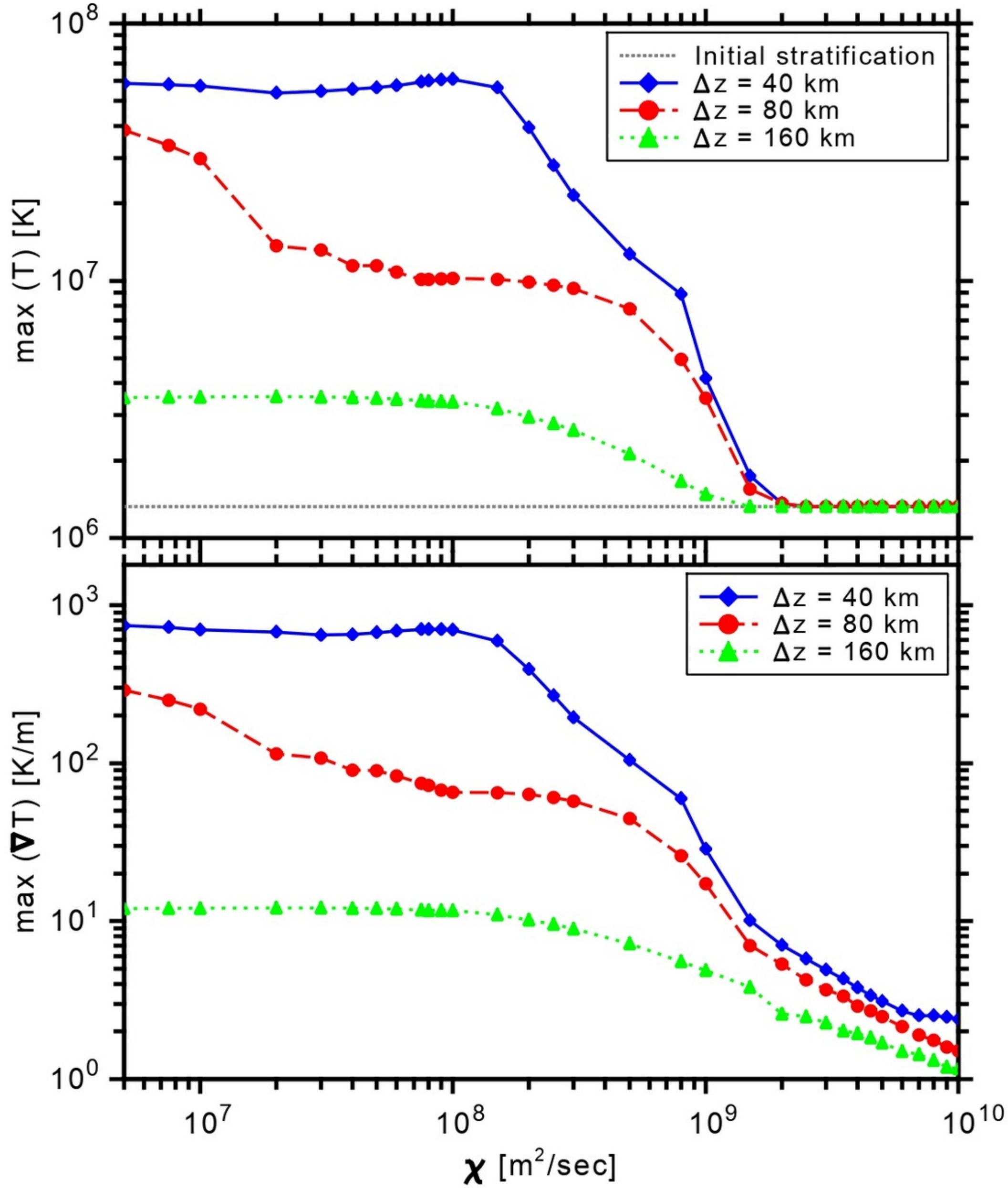
Scaling the heat conduction:



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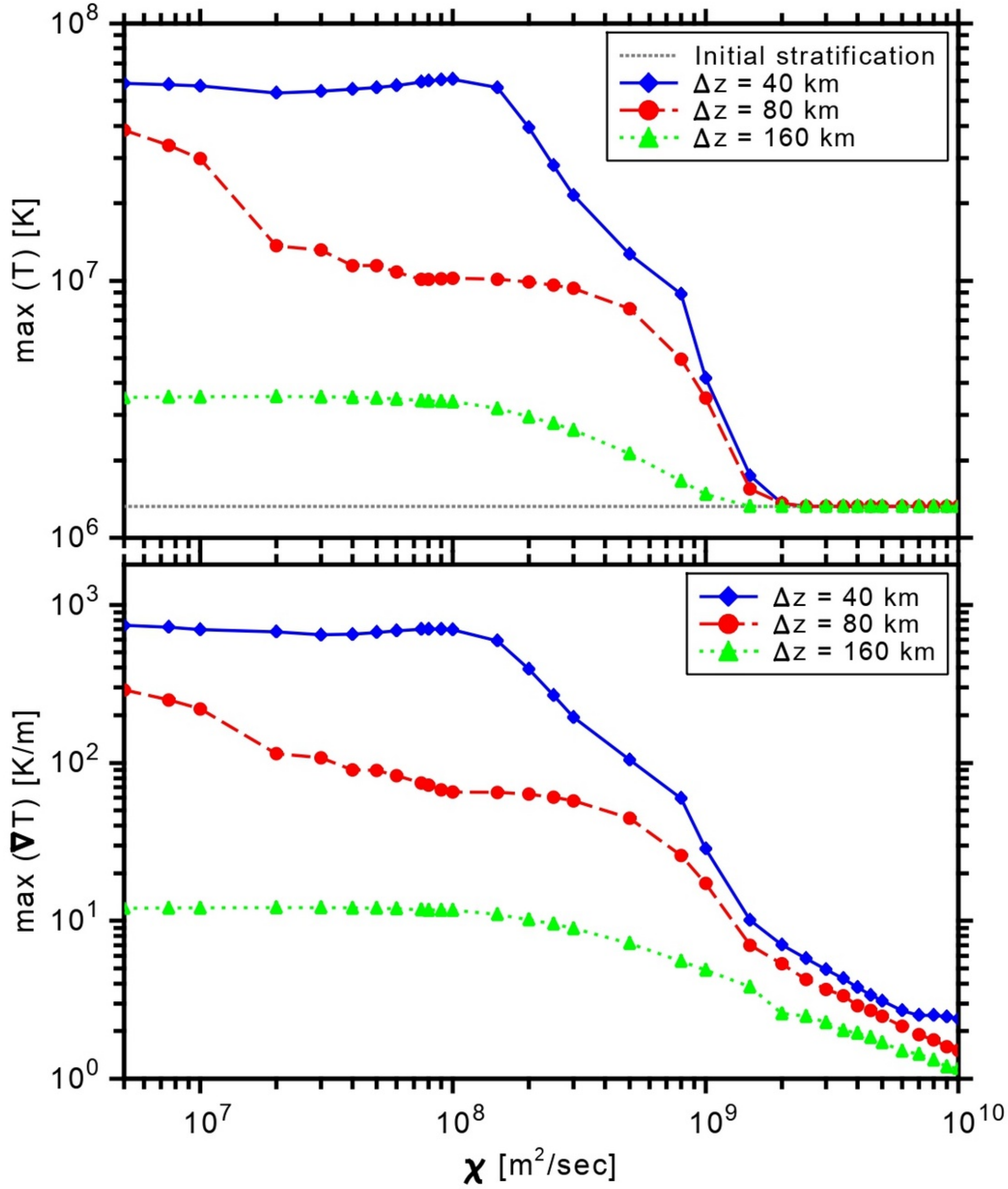
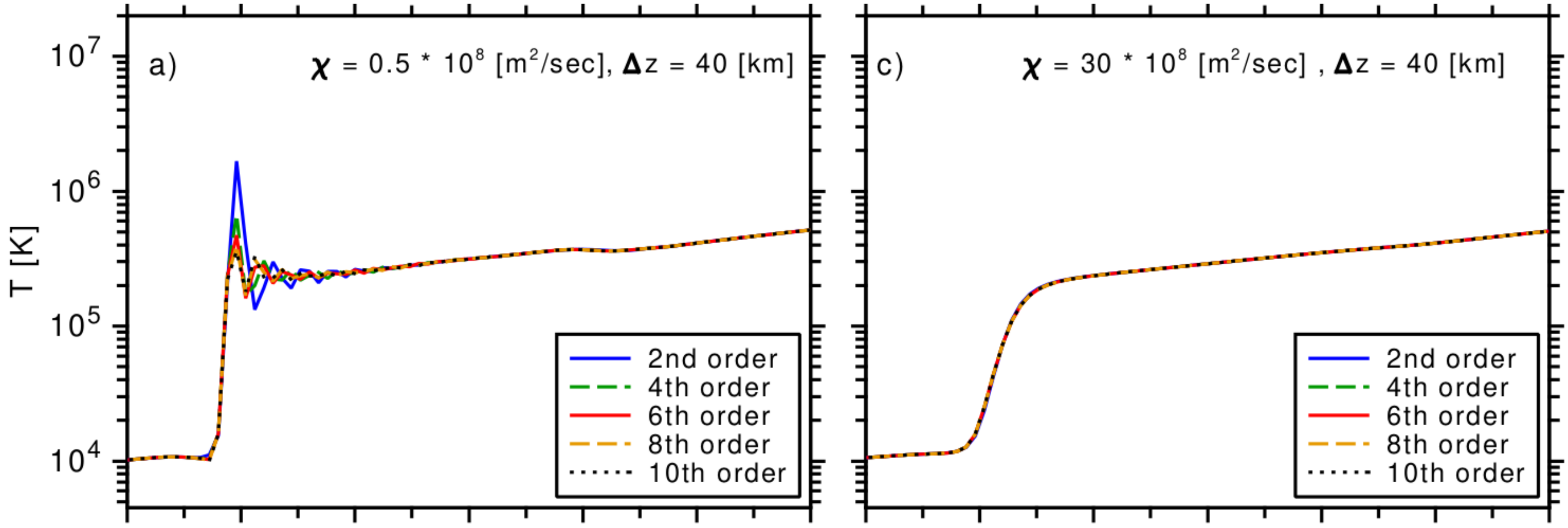


=> higher resolutions do not always imply models are “better”

=> diffusion constants need to fit to the grid resolution

(Pandey & Bourdin, 2025)

Effects due to the order of numerical derivatives:



Pandey & Bourdin (2025)

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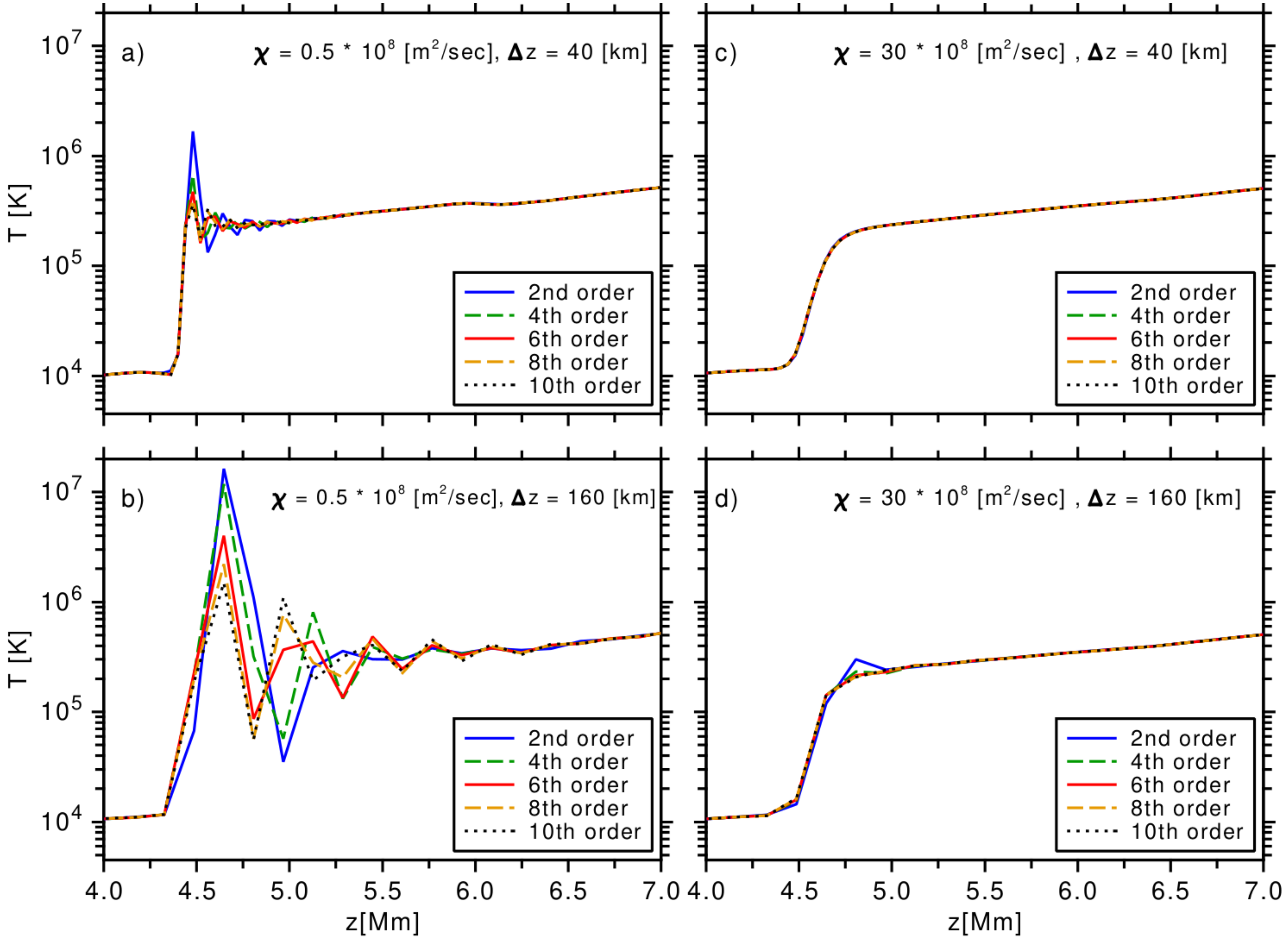

Pandey & Bourdin (2025)

Numerical curiosities
(due to precision & truncation errors)

Precision and machine epsilon

Numerical curiosities cabinet:

$$(x+y)+z \neq x+(y+z)$$

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Machine epsilon:

$$1.0+\epsilon=1.0$$

Precision and machine epsilon

Numerical curiosities cabinet:

$$(x+y)+z \neq x+(y+z)$$

Machine epsilon:

$$1.0+\epsilon=1.0 \qquad (*)$$

- Estimation of the granularity:

(***b = 2; p₀ = 0.5***)

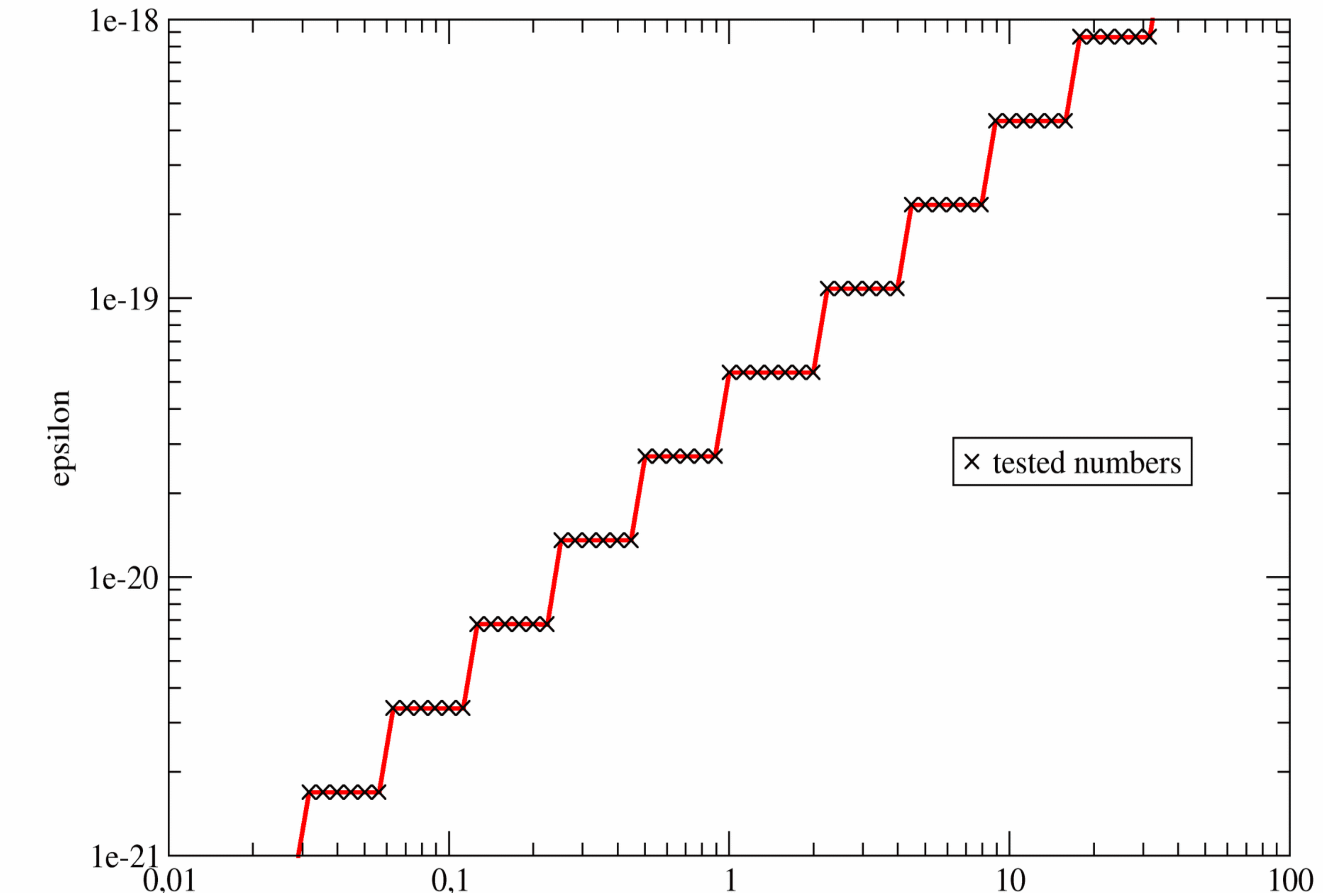
$$\epsilon_N=\frac{b}{2}\cdot b^{-p_N}$$

$$p_{N+1}=p_N\cdot b$$

Stop, if (*) is true

Precision and machine epsilon

Machine epsilon in Fortran 90 (double precision):



Granularity of numbers

Numerical curiosities cabinet: **(continued...)**

Example: simple increment of simulation time:

$$T_N + dT = T_{N+1}$$

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$$4096 + 4 \cdot 10^{-4} = 4096$$

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Example: simple increment of simulation time:

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$$4096 + 4 \cdot 10^{-4} = 4096$$

$$\Rightarrow \frac{T_N}{dT} \approx 10^{-7}$$

Granularity of numbers

Numerical curiosities cabinet: **(continued...)**

<u>Example:</u> simple increment of simulation time:

$$T_N + dT = T_{N+1}$$

$$4096 + 4 \cdot 10^{-4} = 4096$$

$$\Rightarrow \frac{T_N}{dT} \approx 10^{-7}$$

<u>But:</u>

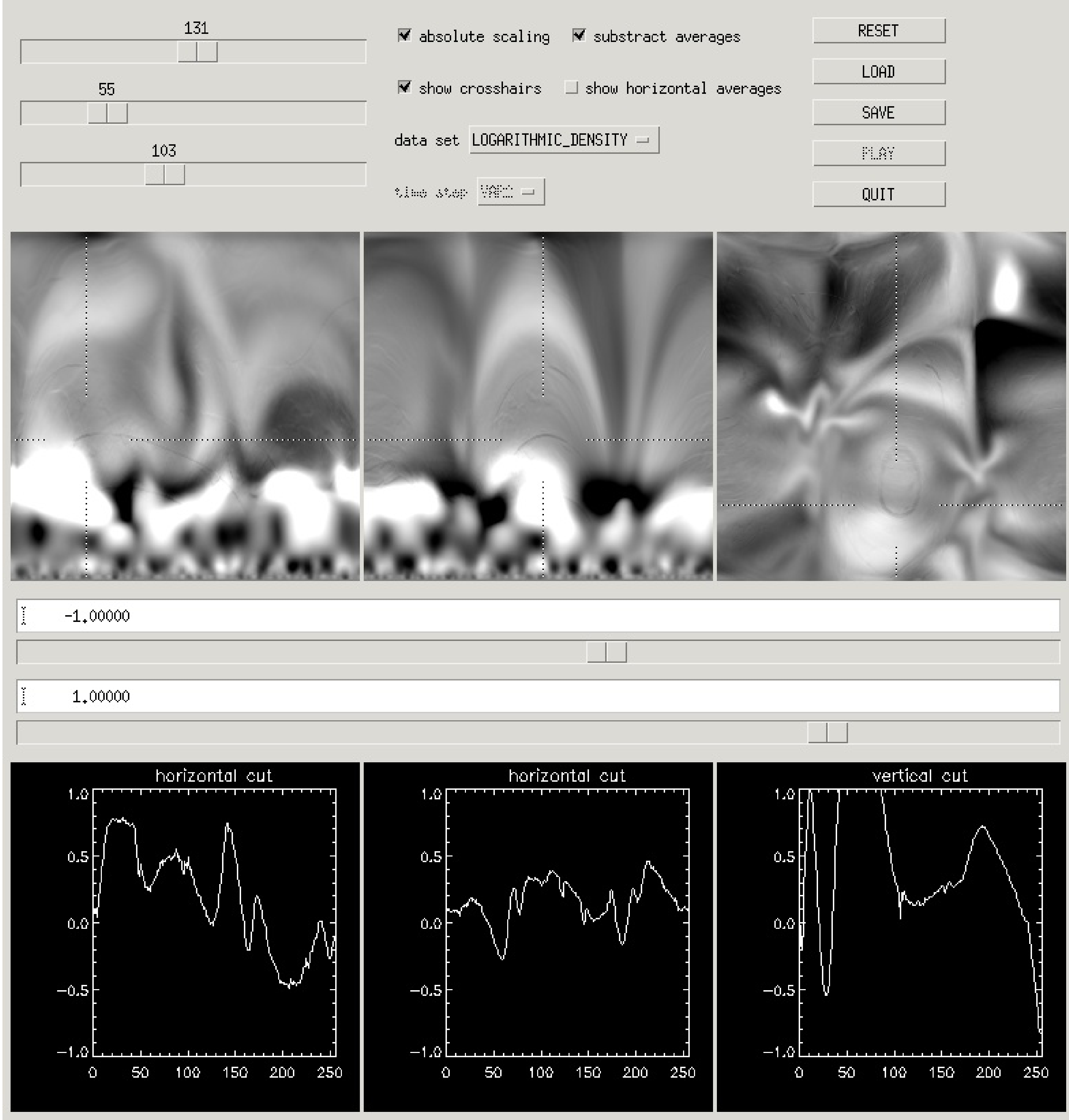
$$4096 + 8 \cdot 10^{-4} \neq 4096$$

Granularity effects in physical observables

Density in a coronal 3D MHD simulation:

ln(ρ):

SP


131
55
103
absolute scaling
substract averages
show crosshairs
show horizontal averages
data set LOGARITHMIC_DENSITY
RESET
LOAD
SAVE
PLAY
QUIT
-1.00000
1.00000
horizontal cut
horizontal cut
vertical cut
1.0
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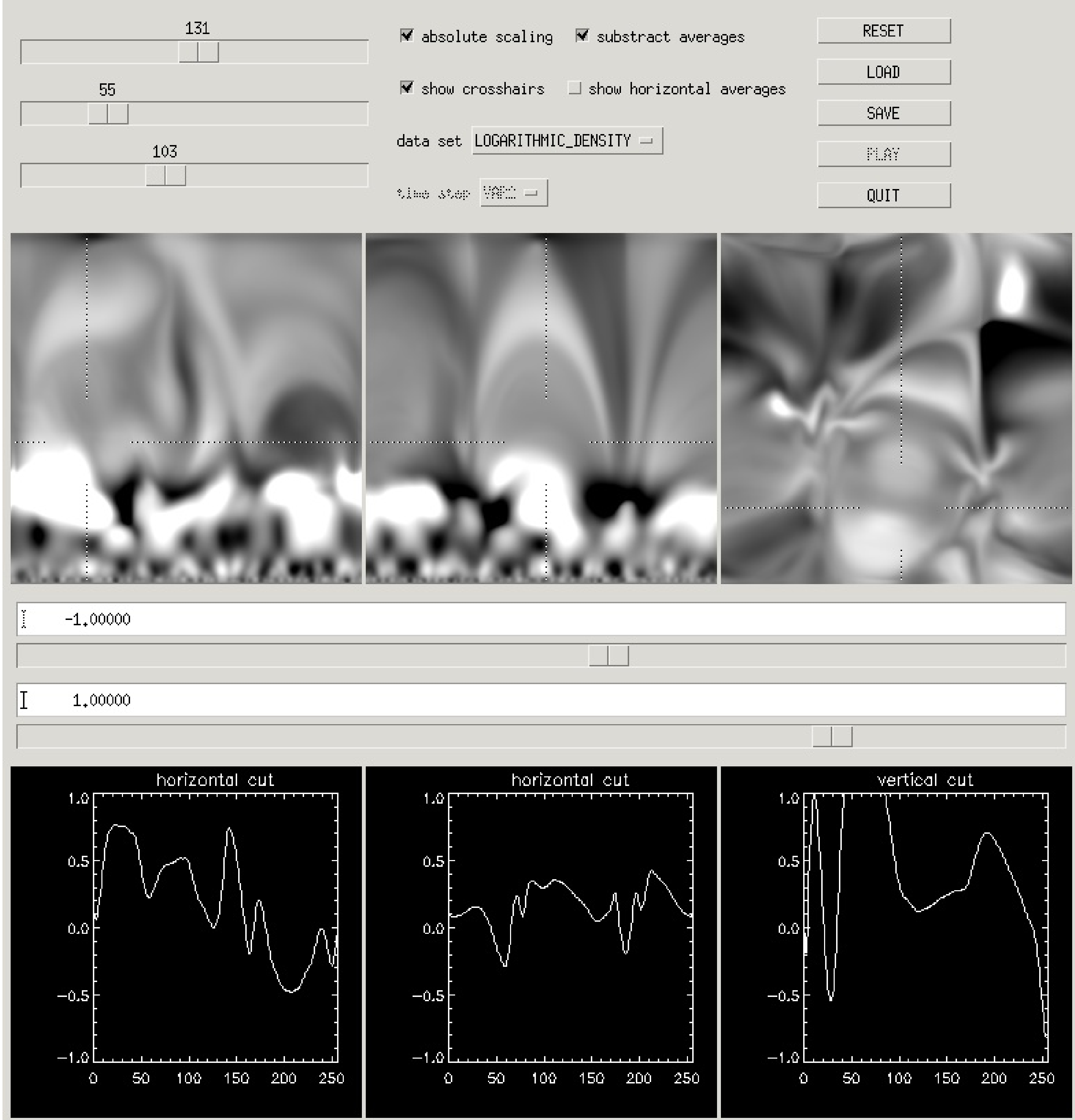
0.0
−0.5
−1.0
0
50
100
150
200
250

ln(ρ):

DP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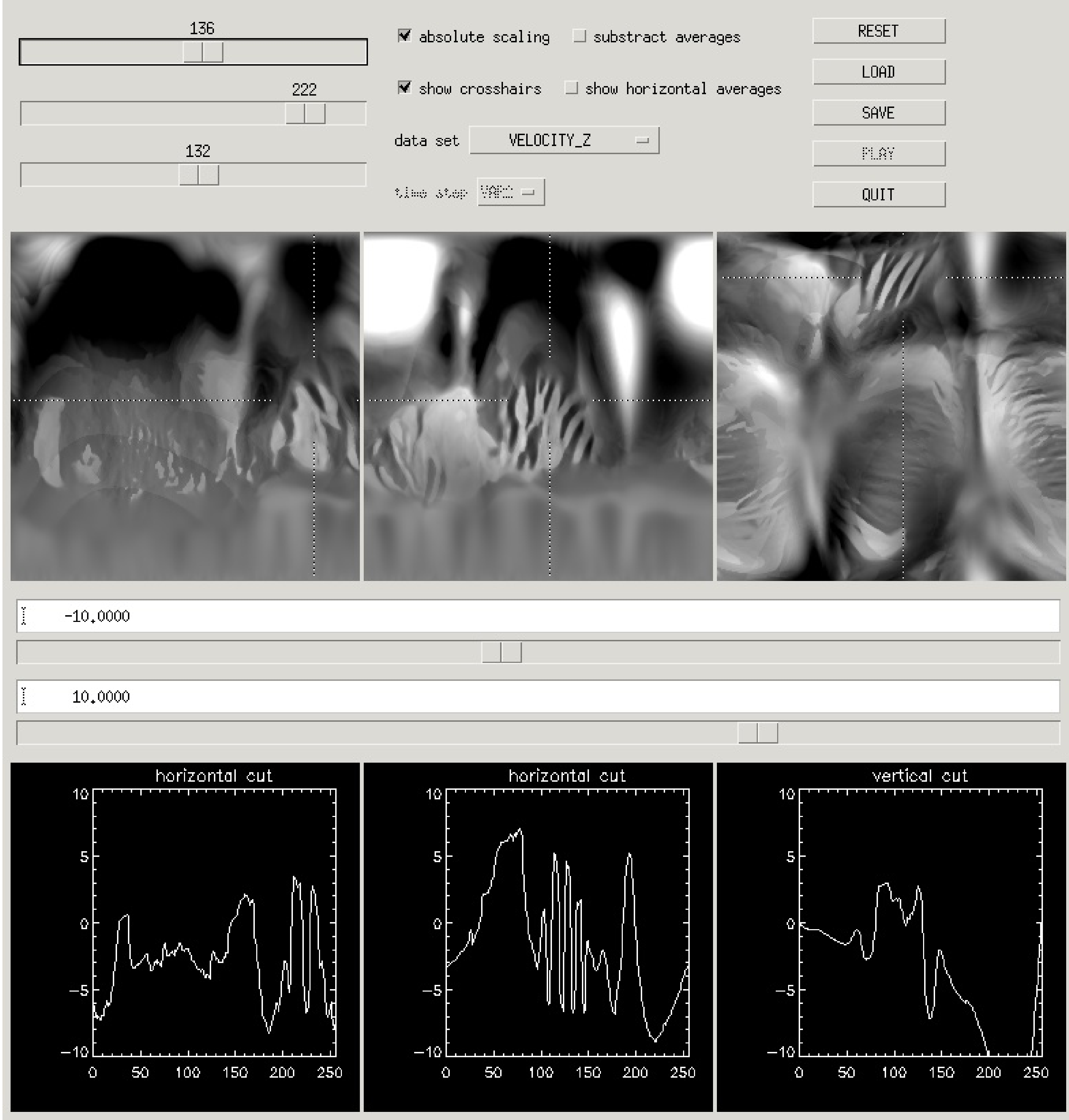
1.0
0.5
0.0
−0.5
−1.0
0
50
100
150
200
250

Granularity effects in physical observables

Vertical velocity:

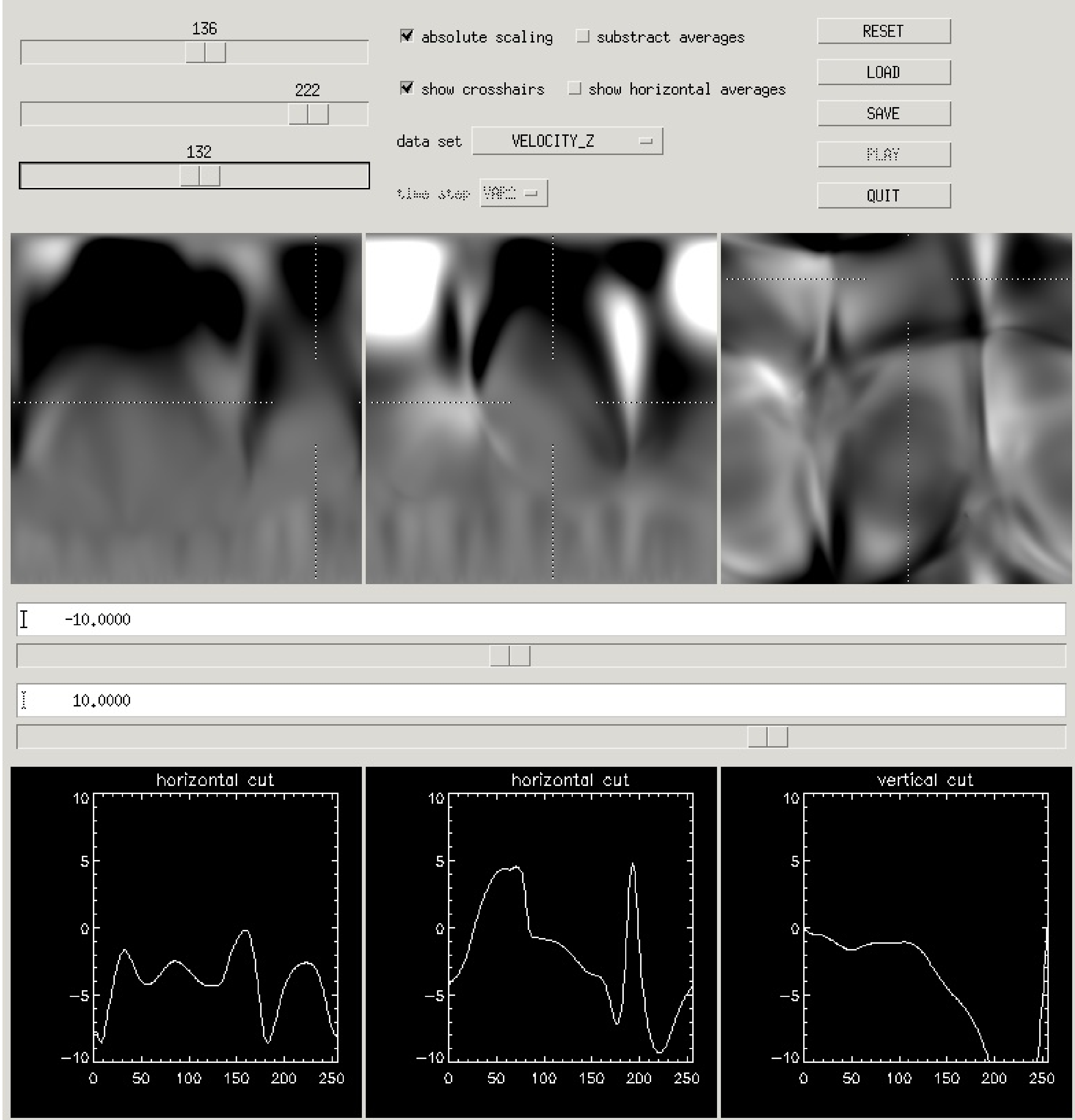
Vz:

SP


136
222
132
absolute scaling
substract averages
show crosshairs
show horizontal averages
data set
VELOCITY_Z
RESET
LOAD
SAVE
PLAY
QUIT
-10.0000
10.0000
horizontal cut
horizontal cut
vertical cut
10
5
0
−5
−10
0
50
100
150
200
250

Vz:

DP



136
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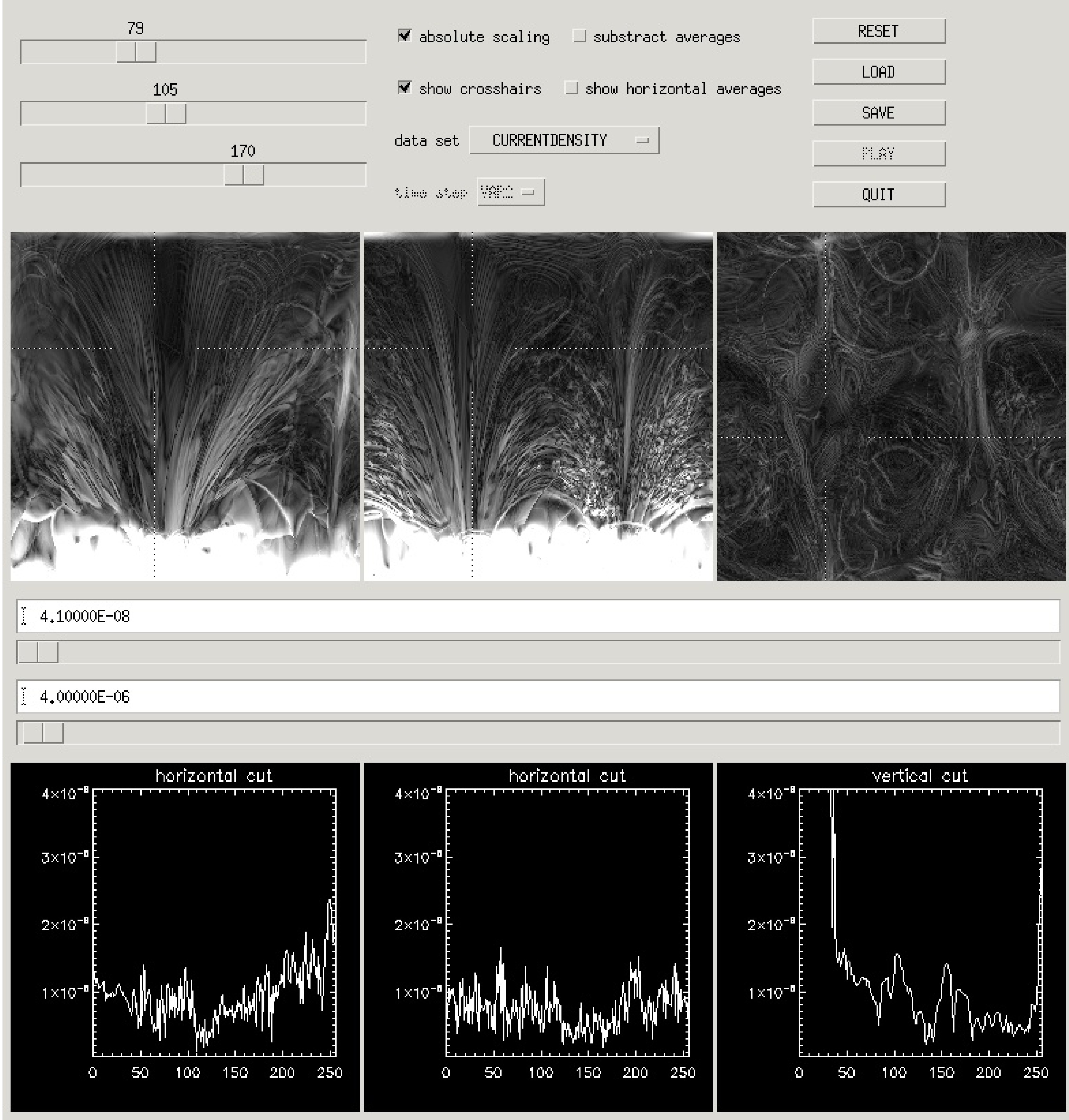
VELOCITY_Z
RESET
LOAD
SAVE
PLAY
QUIT
-10.0000
10.0000
horizontal cut
horizontal cut
vertical cut

Granularity effects in physical observables

Current density / Heating rate: $H = \mu_0 \eta \, \boldsymbol{j}^2 \sim \nabla \times \left(\nabla \times A \right)$

|j|:

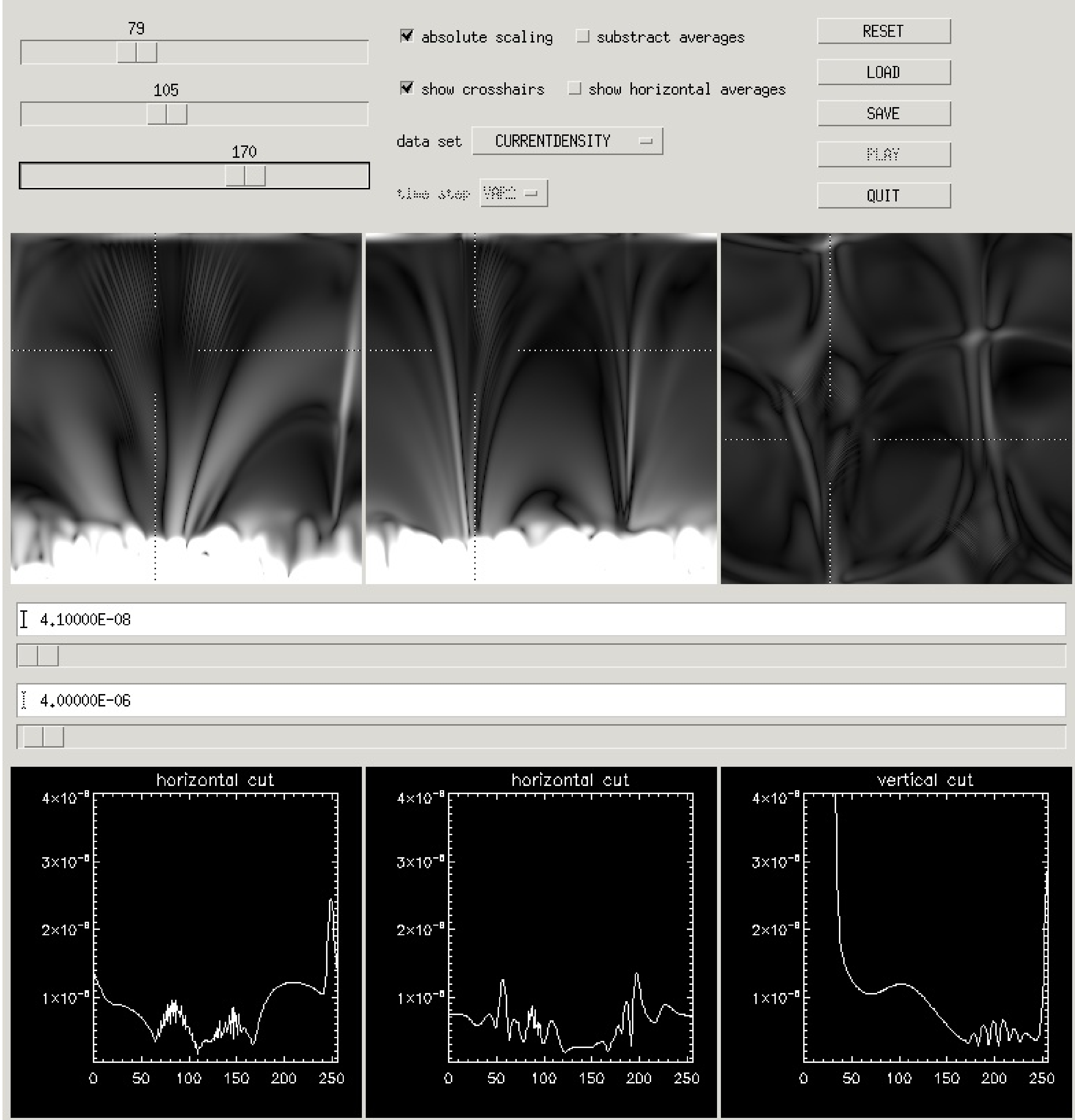
SP



79
105
170
absolute scaling
substract averages
show crosshairs
show horizontal averages
data set
CURRENTDENSITY
RESET
LOAD
SAVE
PLAY
QUIT
4.10000E-08
4.00000E-06
horizontal cut
horizontal cut
vertical cut
4×10⁻⁸
3×10⁻⁸
2×10⁻⁸
1×10⁻⁸
0
50
100
150
200
250

|j|:

DP



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horizontal cut
horizontal cut
vertical cut
4×10⁻⁸
3×10⁻⁸
2×10⁻⁸
1×10⁻⁸
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Catastrophic cancellation:

“What Every Computer Scientist Should Know About Floating-Point Arithmetic”

(David Goldberg, 1991)

$$\boldsymbol{\nabla} \times \boldsymbol{A} \sim \boldsymbol{B} \quad ; \quad \boldsymbol{\nabla} \times \boldsymbol{B} \sim \boldsymbol{j}$$

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$$j_Z \sim \frac{\partial B_Y}{\partial x} - \frac{\partial B_X}{\partial y}$$

$$B_X \approx B_Y$$

Catastrophic cancellation:

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Granularity effects in physical observables

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$$\Rightarrow \quad j_Z \approx 2 \cdot \epsilon$$

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Problem: initial condition might not be in „numerical equilibrium“

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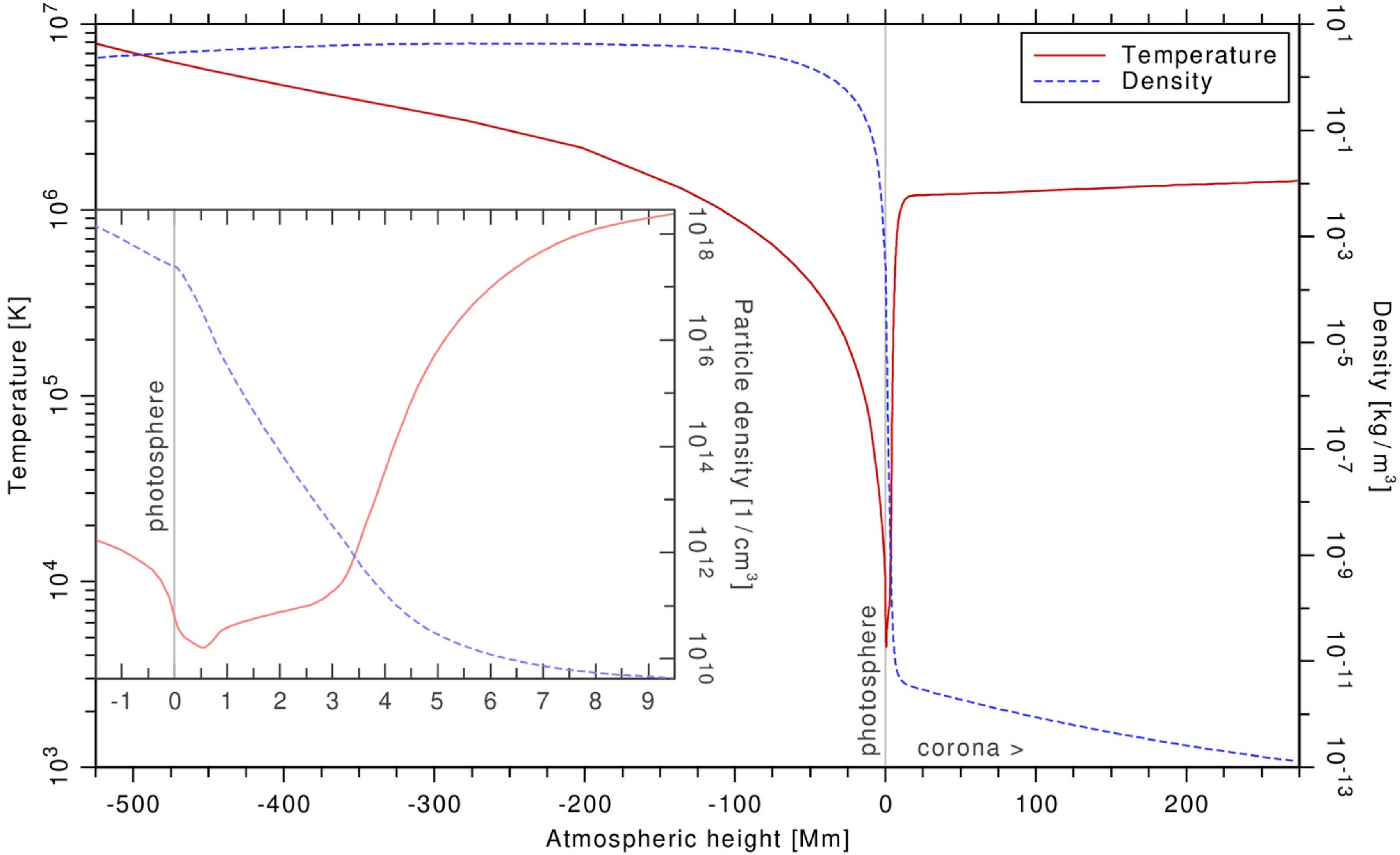

=> Solar atmosphere in hydrostatic equilibrium (Bourdin, 2014, CEAB)

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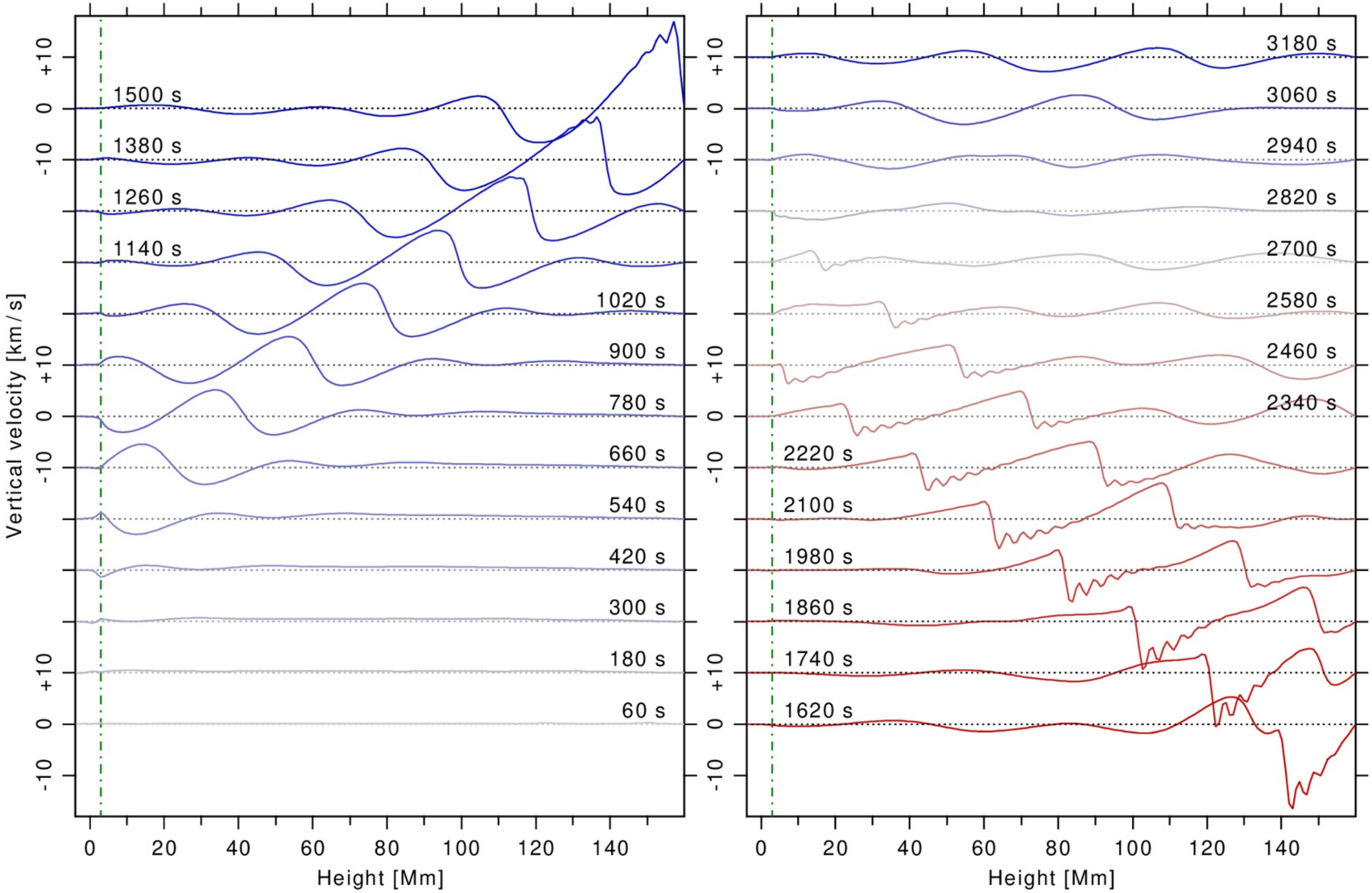

=> Analytic solution needs time to equilibrate (Bourdin, 2014, CEAB)

Driving a simulation with external forces

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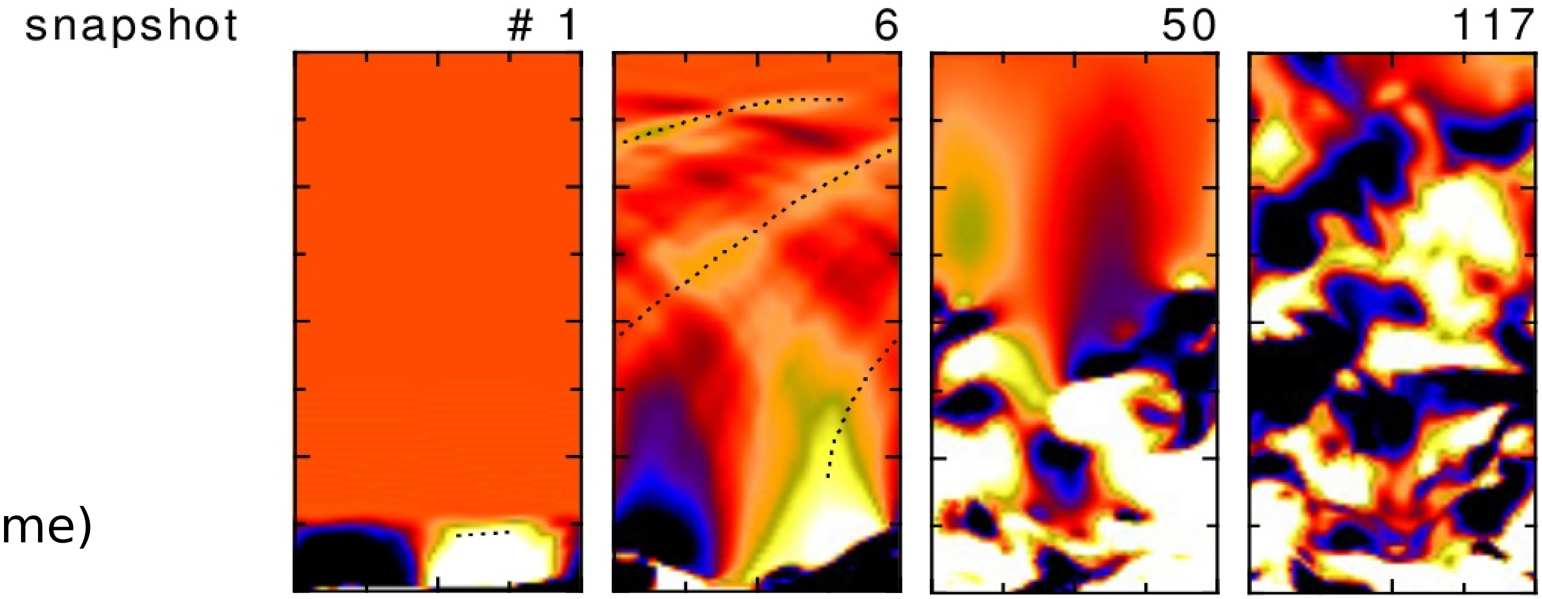

(samples/
turbulent_flame)

(Bourdin, 2014, CEAB, 38, 1–10)

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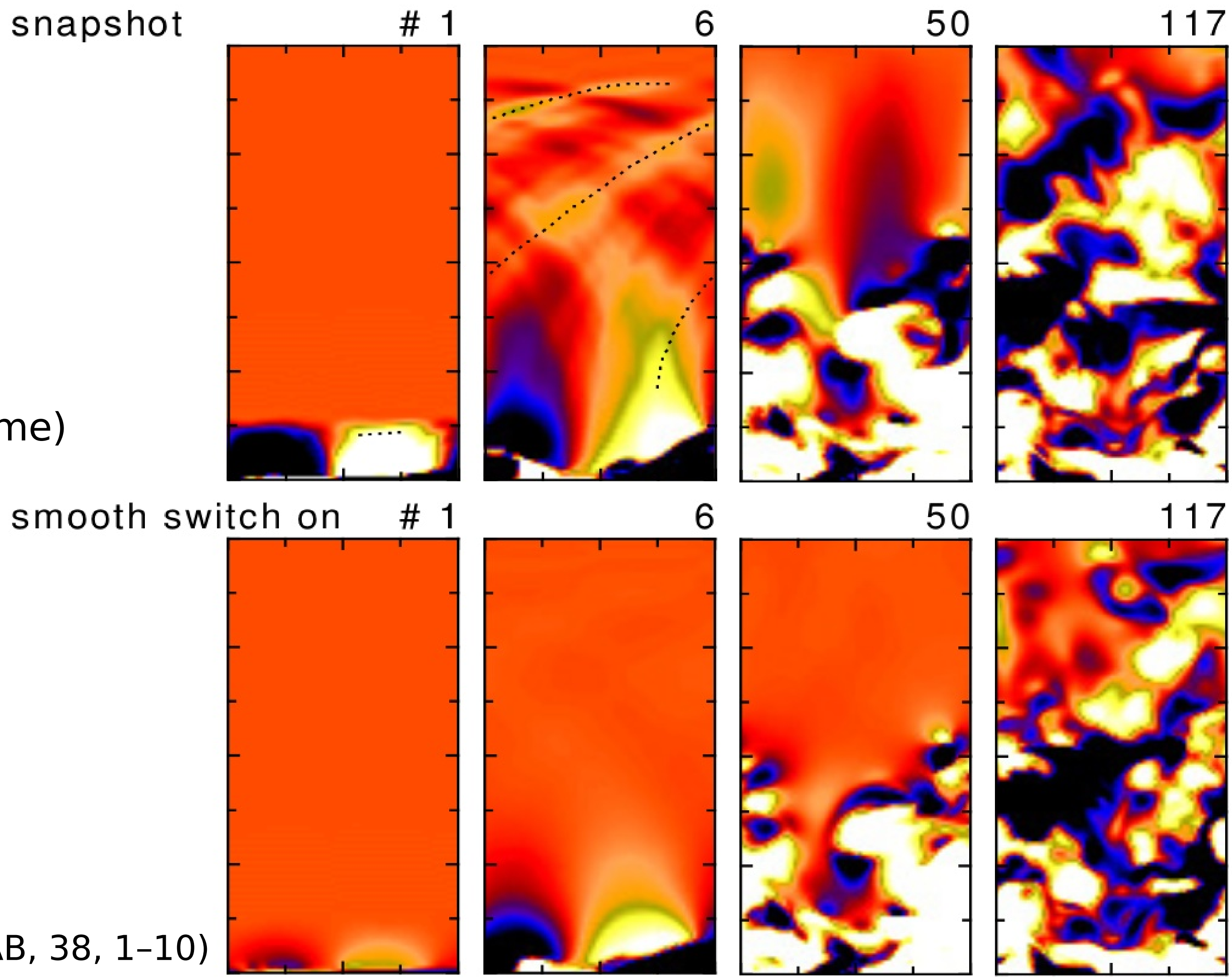

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