Multilevel 3D NLTE modeling with the code PORTA

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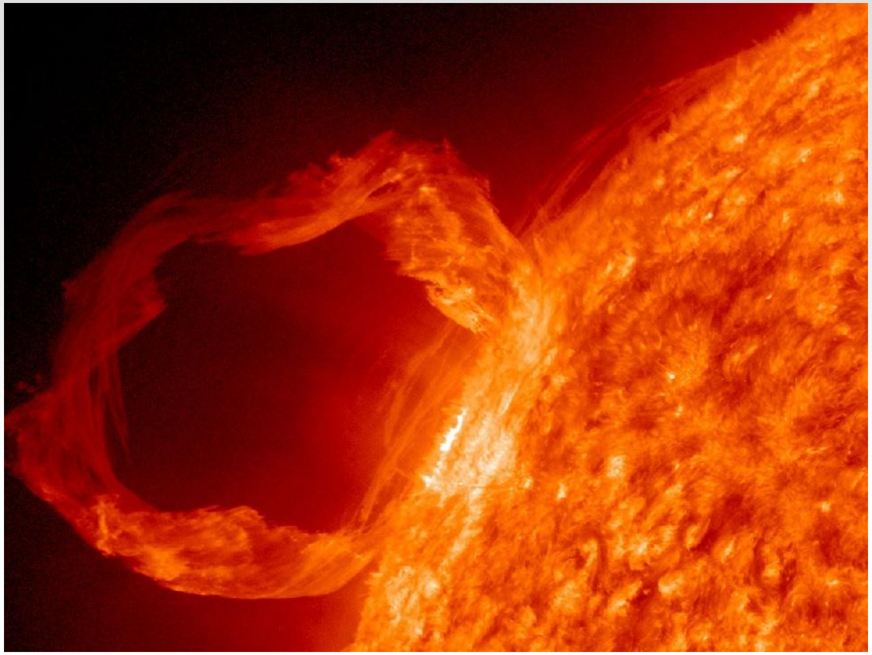
The complexity of the solar atmosphere



Solar observations:

Spatial resolution: ~100 km
Polarimetric sensitivity: 10^{-5}
High spectral resolution

Very broad range of physical conditions within few Mm:
>10 orders of magnitude in density
~3 orders of magn. in temperature
LTE, NLTE, optically thin

We understand the interior much better than the atmosphere.

Why, in which regions, and how do we need 3D radiative transfer modeling?

Line formation regimes

Average quiet atmosphere (VAL-C)

LTE

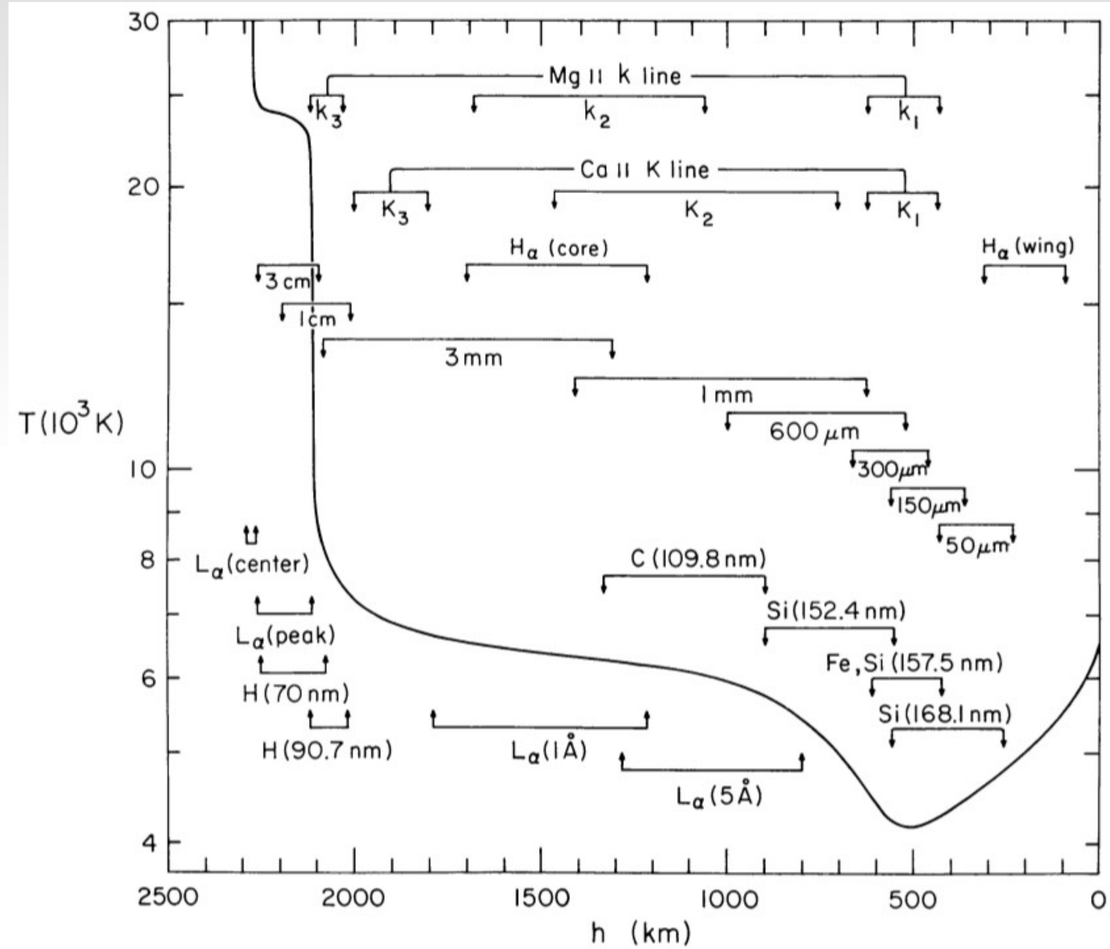
Collisions lead to Boltzmann atomic populations

Optically thin plasma

Boundary illumination + Collisions

NLTE (non-LTE)

General case of non-local coupling of plasma conditions by radiation



(Vernazza et al., 1981)

The equations of the NLTE problem

Two sets of equations (**CRD limit**):

(1) Statistical equilibrium equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^K_Q(\alpha J) = -2\pi\mathrm{i}\,\nu_\mathrm{L}\,g_{\alpha J}\,Q\,\rho^K_Q(\alpha J)$$
$$+\sum_{\alpha_\ell J_\ell}\sum_{K_\ell Q_\ell}\rho^{K_\ell}_{Q_\ell}(\alpha_\ell J_\ell)\,\mathbb{T}_\mathrm{A}(\alpha JKQ,\alpha_\ell J_\ell K_\ell Q_\ell)+$$
$$+\sum_{\alpha_u J_u}\sum_{K_u Q_u}\rho^{K_u}_{Q_u}(\alpha_u J_u)\Big[\mathbb{T}_\mathrm{E}(\alpha JKQ,\alpha_u J_u K_u Q_u)$$
$$+\mathbb{T}_\mathrm{S}(\alpha JKQ,\alpha_u J_u K_u Q_u)\Big]$$
$$-\sum_{K'Q'}\rho^{K'}_{Q'}(\alpha J)\Big[\mathbb{R}_\mathrm{A}(\alpha JKQK'Q')+\mathbb{R}_\mathrm{E}(\alpha JKQK'Q')$$
$$+\mathbb{R}_\mathrm{S}(\alpha JKQK'Q')\Big]$$

$$+\ \text{collisional rates}$$

(2) Radiative transfer equation

$$\eta_i^\mathrm{A}(\nu,\vec\Omega) = \frac{h\nu}{4\pi}\mathcal{N}\sum_{\alpha_\ell J_\ell}\sum_{\alpha_u J_u}(2J_\ell+1)\,B(\alpha_\ell J_\ell\to\alpha_u J_u)$$
$$\times\sum_{KQK_\ell Q_\ell}\sqrt{3(2K+1)(2K_\ell+1)}\ \times$$
$$\times\sum_{M_\ell M_\ell' M_u qq'}(-1)^{1+J_\ell-M_\ell+q'}\begin{pmatrix}J_u & J_\ell & 1\\ -M_u & M_\ell & -q\end{pmatrix}\begin{pmatrix}J_u & J_\ell & 1\\ -M_u & M_\ell' & -q'\end{pmatrix}$$
$$\times\begin{pmatrix}1 & 1 & K\\ q & -q' & -Q\end{pmatrix}\begin{pmatrix}J_\ell & J_\ell & K_\ell\\ M_\ell & -M_\ell' & -Q_\ell\end{pmatrix}$$
$$\times\,\mathrm{Re}\Big[\mathcal{T}^K_Q(i,\vec\Omega)\ \rho^{K_\ell}_{Q_\ell}(\alpha_\ell J_\ell)\ \Phi(\nu_{\alpha_u J_u M_u,\,\alpha_\ell J_\ell M_\ell}-\nu)\Big]$$

$$\eta_i^\mathrm{S}(\nu,\vec\Omega) = \frac{h\nu}{4\pi}\mathcal{N}\sum_{\alpha_\ell J_\ell}\sum_{\alpha_u J_u}(2J_u+1)\,B(\alpha_u J_u\to\alpha_\ell J_\ell)$$
$$\times\sum_{KQK_u Q_u}\sqrt{3(2K+1)(2K_u+1)}$$
$$\times\sum_{M_u M_u' M_\ell qq'}(-1)^{1+J_u-M_u+q'}\begin{pmatrix}J_u & J_\ell & 1\\ -M_u & M_\ell & -q\end{pmatrix}\begin{pmatrix}J_u & J_\ell & 1\\ -M_u' & M_\ell & -q'\end{pmatrix}$$
$$\times\begin{pmatrix}1 & 1 & K\\ q & -q' & -Q\end{pmatrix}\begin{pmatrix}J_u & J_u & K_u\\ M_u' & -M_u & -Q_u\end{pmatrix}$$
$$\times\,\mathrm{Re}\Big[\mathcal{T}^K_Q(i,\vec\Omega)\ \rho^{K_u}_{Q_u}(\alpha_u J_u)\ \Phi(\nu_{\alpha_u J_u M_u,\,\alpha_\ell J_\ell M_\ell}-\nu)\Big]$$

$$\rho_i^\mathrm{A}(\nu,\vec\Omega) = \eta_i^\mathrm{A}(\nu,\vec\Omega)\,\big\{\mathrm{Re}\to\mathrm{Im}\big\}$$

$$\rho_i^\mathrm{S}(\nu,\vec\Omega) = \eta_i^\mathrm{S}(\nu,\vec\Omega)\,\big\{\mathrm{Re}\to\mathrm{Im}\big\}$$

$$\varepsilon_i(\nu,\vec\Omega) = \frac{2h\nu^3}{c^2}\ \eta_i^\mathrm{S}(\nu,\vec\Omega)\,.$$

Atomic polarization: $\boldsymbol{\rho^K{}_Q \neq \delta_{K0}\,\delta_{Q0}\,\rho^0{}_0}$

(Landi Degl'Innocenti & Landolfi, 2004)

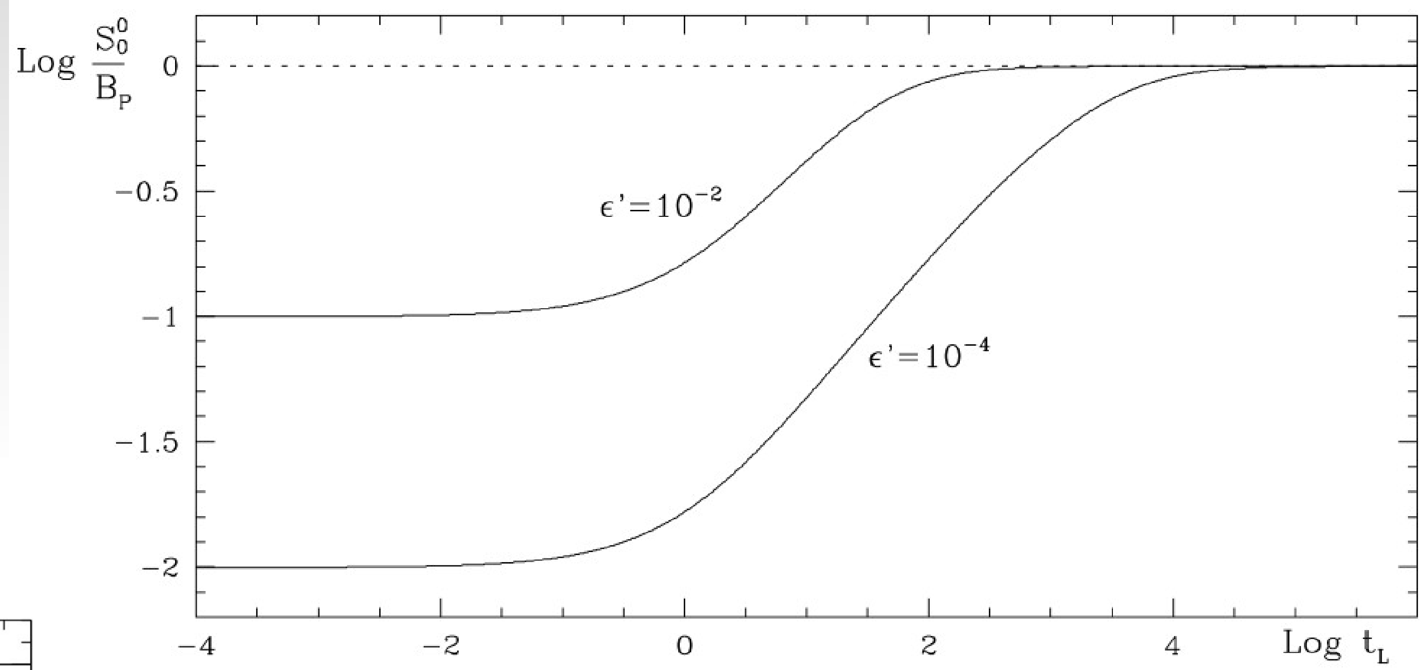
Line formation in the 1D plane-parallel geometry

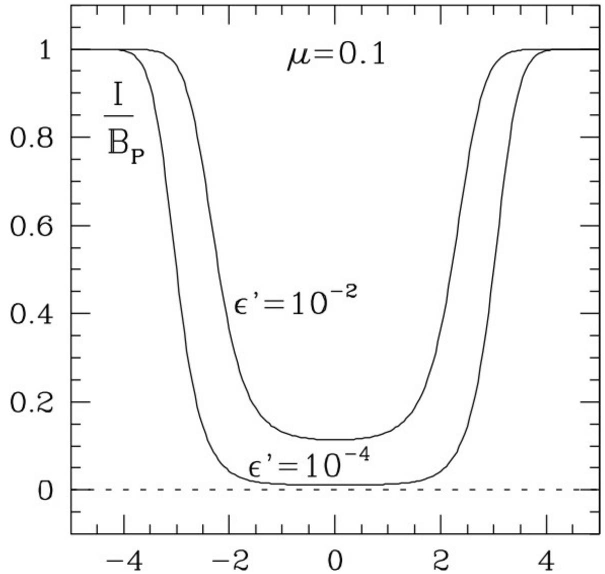
Collisions: Coupling of radiation to local plasma conditions

$\varepsilon = C_{ul} / (C_{ul} + A_{ul})$

Atomic state near the surface of the atmosphere: far from thermal equilibrium

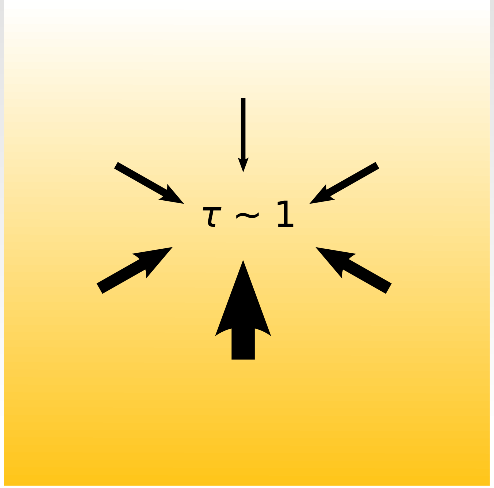
The line source function: $S = \epsilon / \eta$



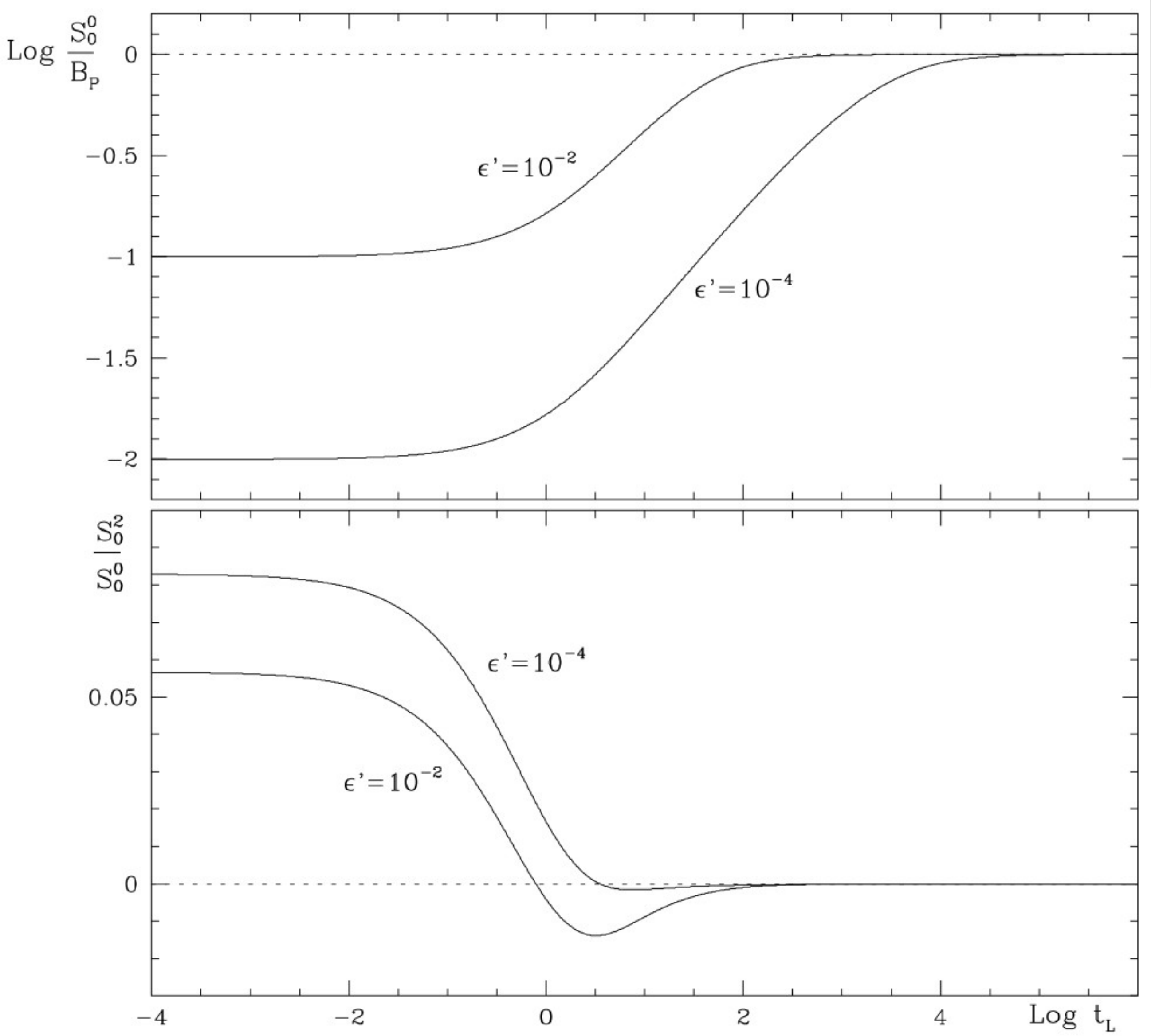


Height variation of ***S*** determines the spectral line shape

Anisotropy of radiation

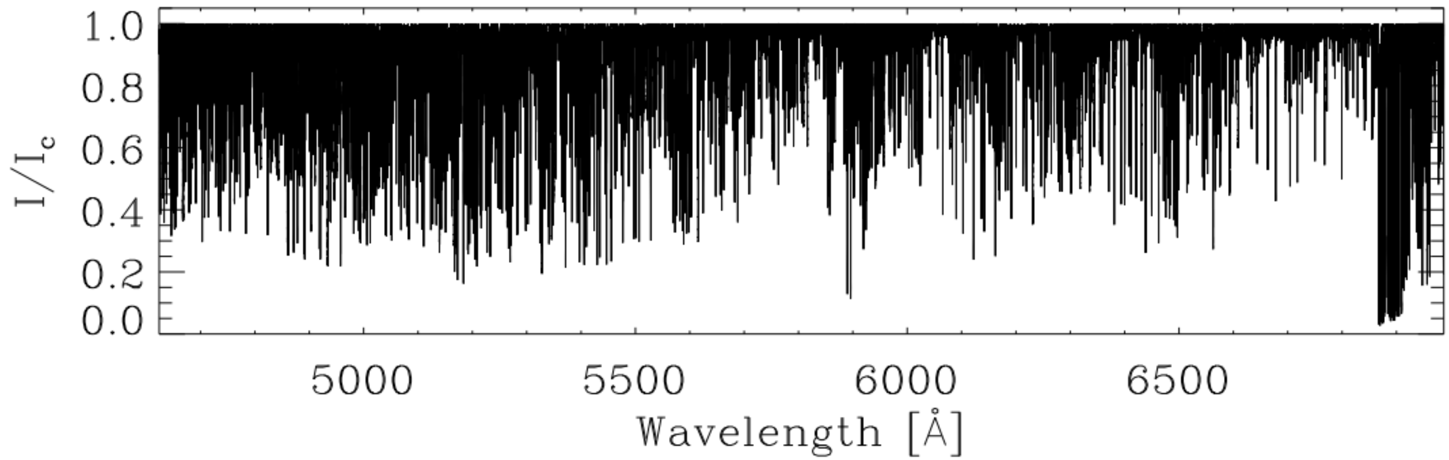


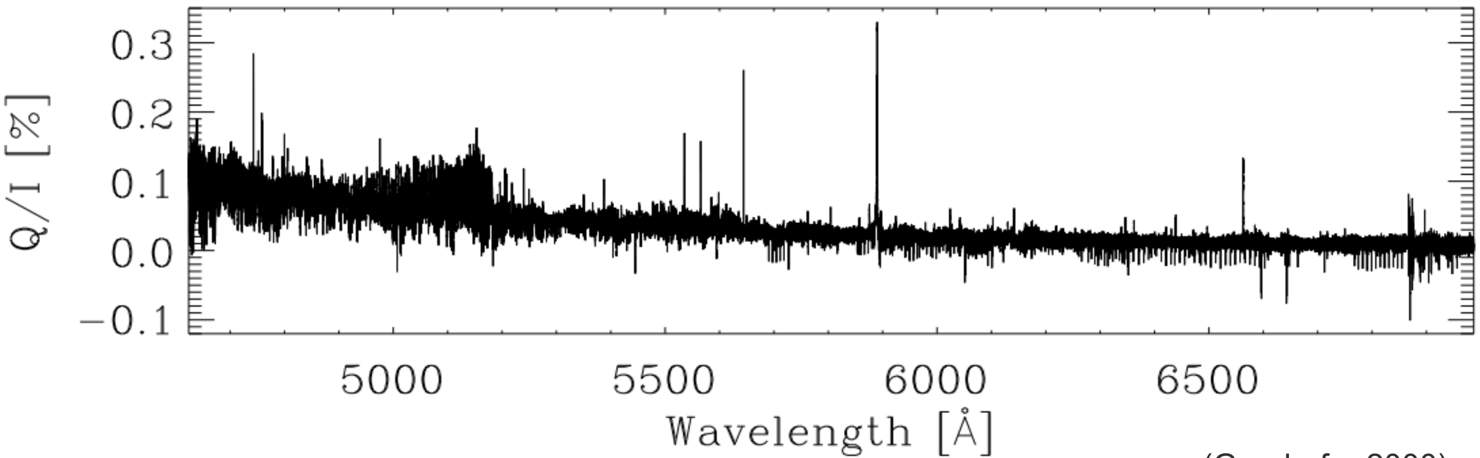
Anisotropy of radiation induces **atomic polarization** that can be further modified by the **Hanle effect.**



The Second Solar Spectrum

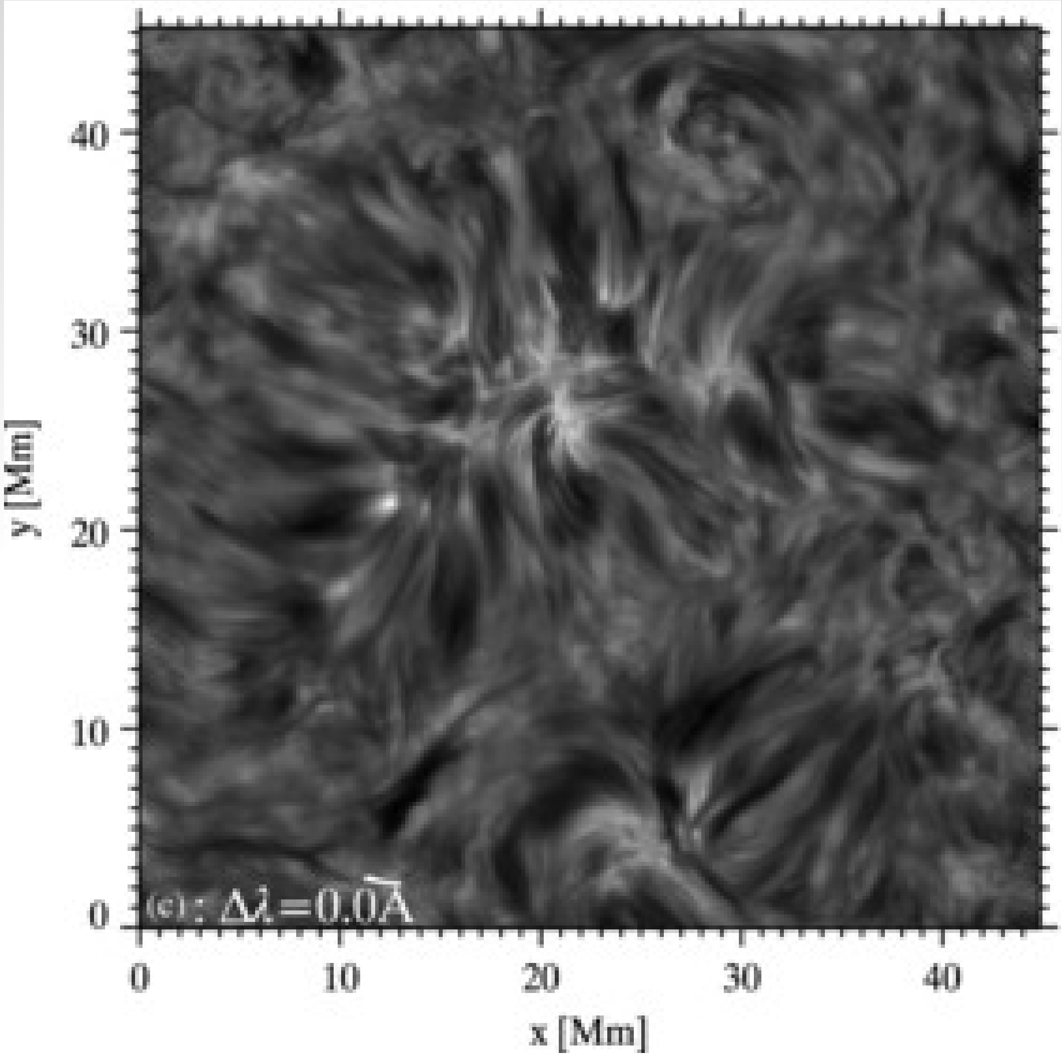
No spatial resolution of the observation → Spectral lines and continuum near the solar limb show a rich variety of linearly polarized features





(Gandorfer 2000)

Observations with high spatial resolution



(Quiet Sun in H-alpha)

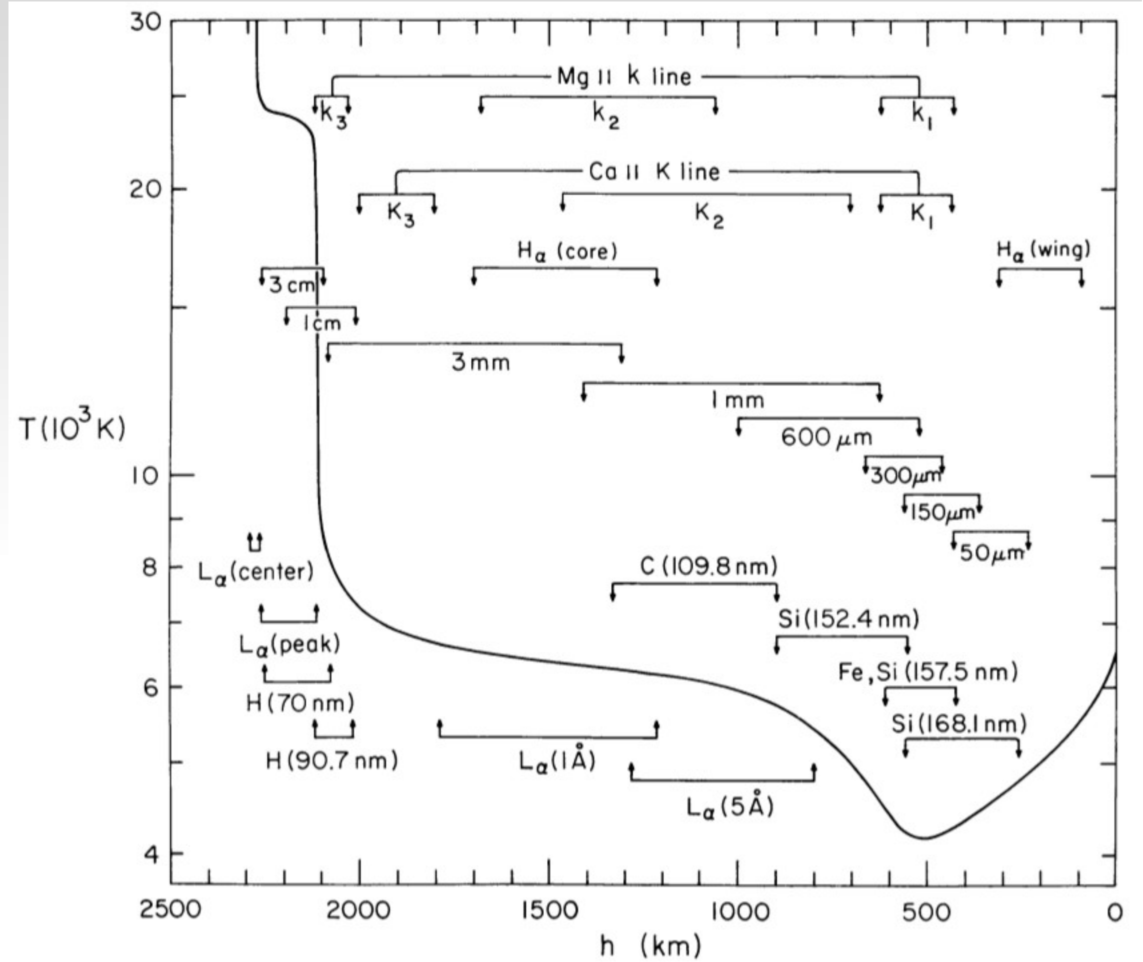
1D plane-parallel models

Semi-empirical hydrostatic 1D plane-parallel models: Based on fitting of the line and continuum intensities.

Different type of structure → different model.

Type of structure observed → We know **a priori** the radiation field anisotropy and we deduce the magnetic field by differential comparison.

Limitations:
No dynamics
No magnetic field
One model cannot fit all the lines



Can the complex 3D structure be approximated by an average 1D model?

A numerical experiment

Isothermal semi-infinite plane-parallel atmosphere (H = 2000 km)

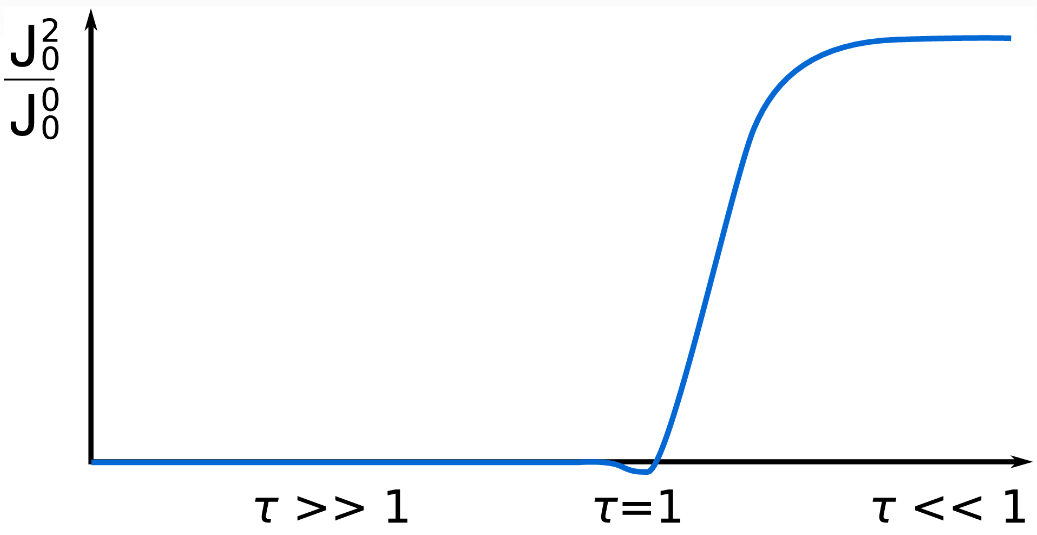
Two-level atom (J_l=0, J_u=1)

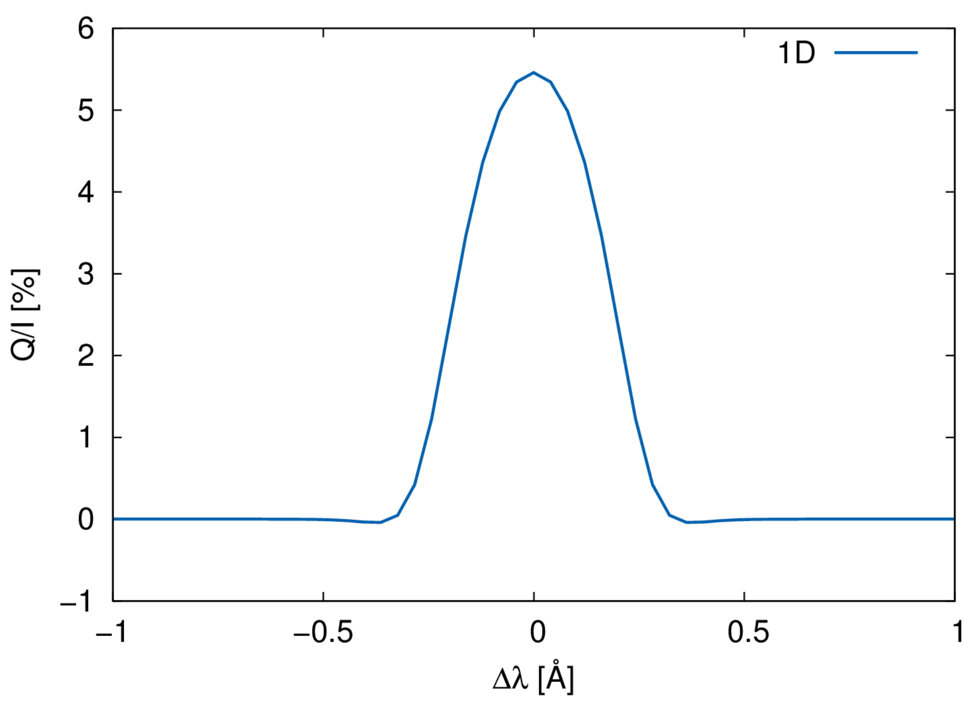
A_{ul} = 10^8 s^{-1}

T = 6000 K

ε = 10^{-4}

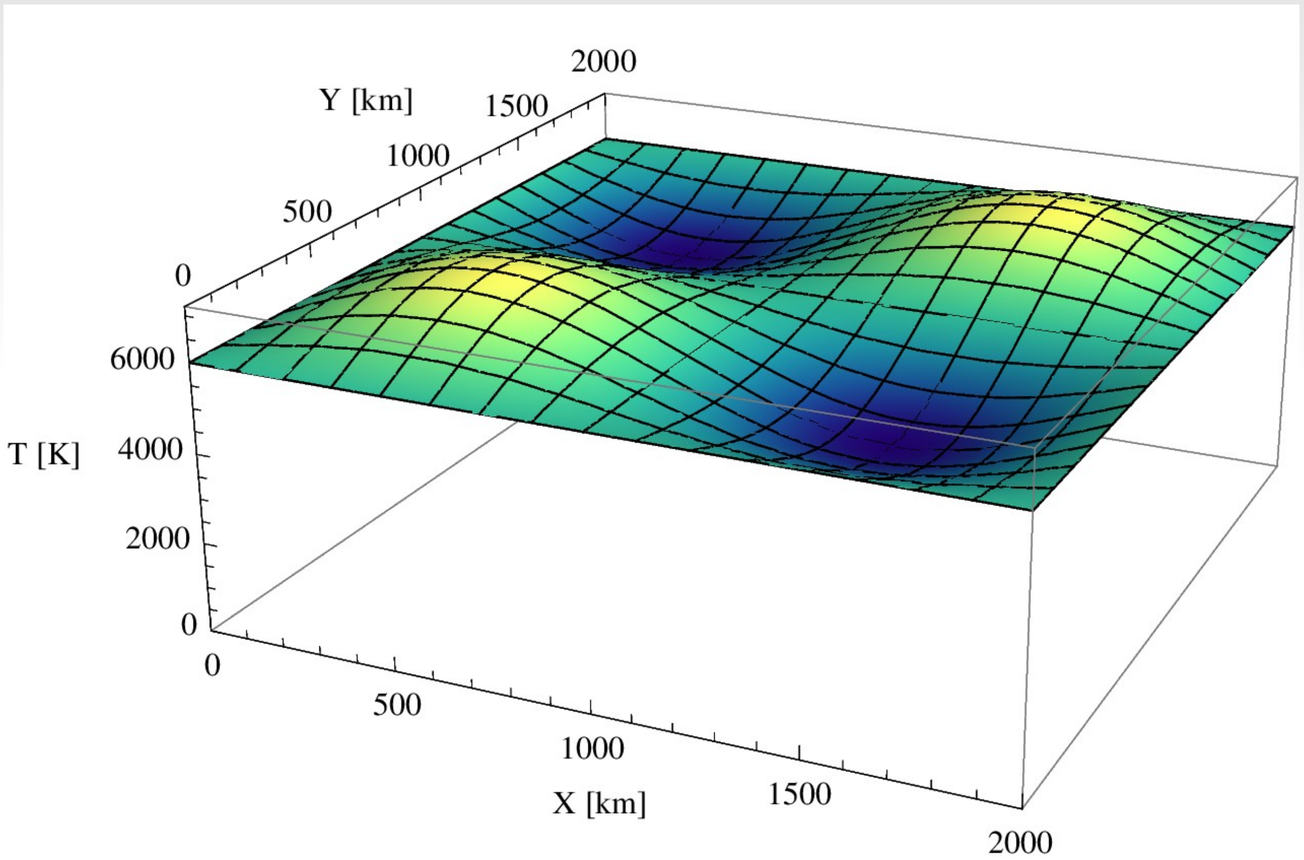
B = 0 G





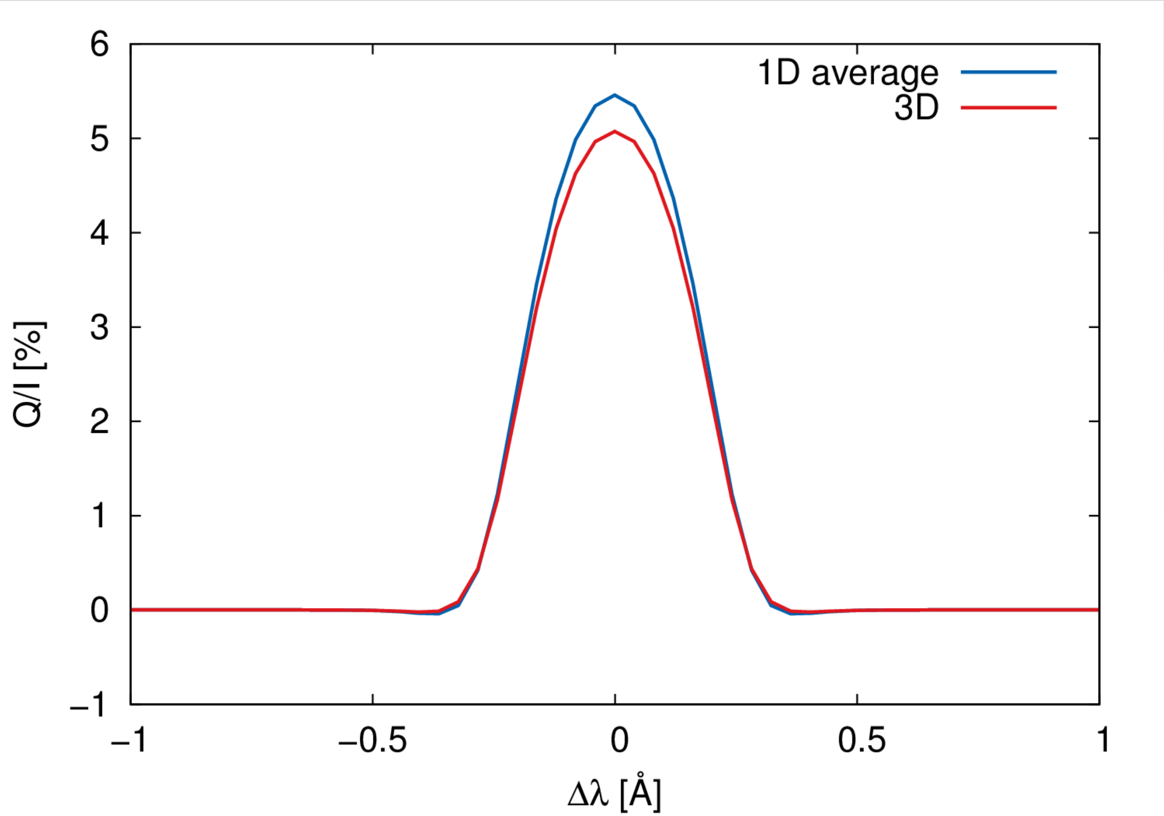
The role of unresolved inhomogeneities

We add a horizontal perturbation of the plasma kinetic temperature
(the **symmetry breaking effect)**:



The horizontally averaged atmosphere is still isothermal.

The role of unresolved inhomogeneities



Symmetry breaking effects: **non-linearly coupled** to the line intensity and polarization.

Neglecting the horizontal inhomogeneities → wrong conclusion on the presence of **~10 G** magnetic field.

1D modeling is generally unsuitable for high-precision diagnostics even in the case of no spatial resolution

The concept of average atmosphere

1D:

average observation → average model atmosphere → diagnostics

Suitable for order-of-magnitude estimates.

Average 1D atmosphere does **not** represent the spatial average of the real atmosphere. (Column-mass scale & multi-component models: Inapplicable in multi-D polarization modeling.)

3D:

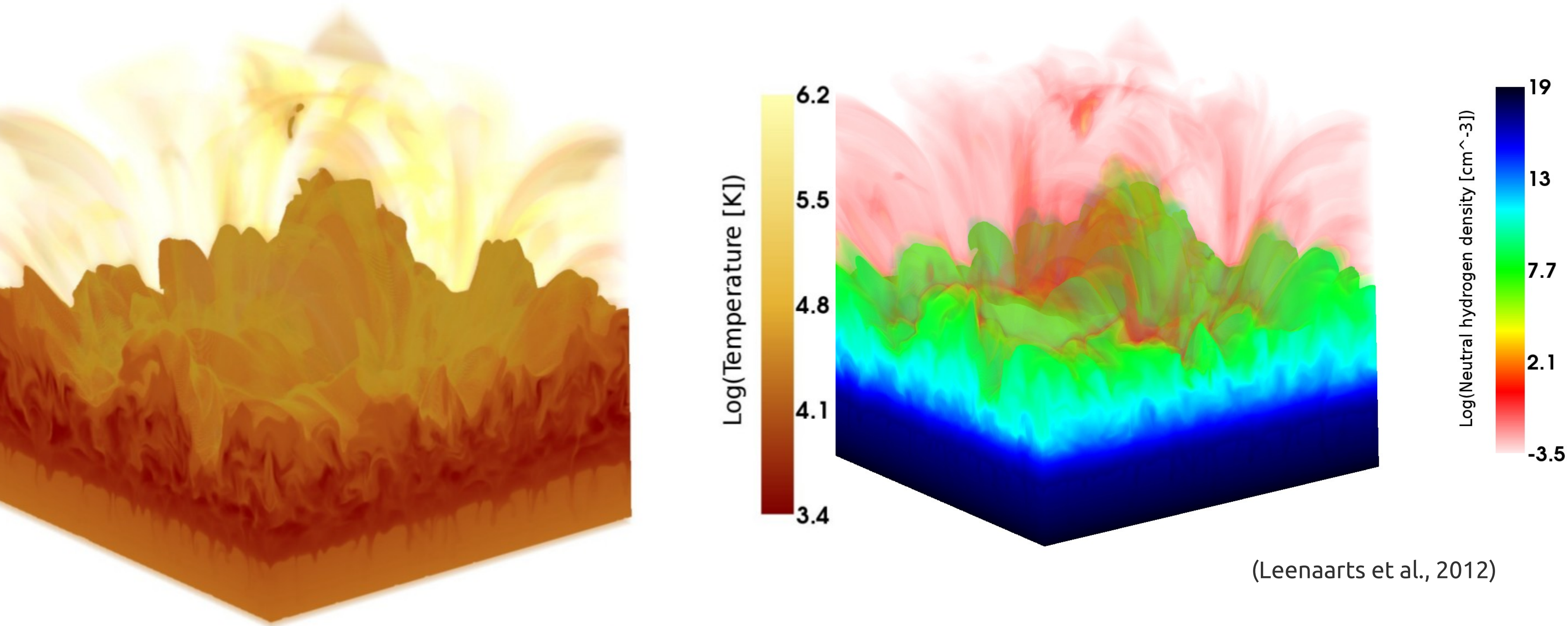
ab initio simulation → 3D model → (average) spectrum

As little of free parameters as possible.
We can still speak about the average atmosphere in 3D: set of sufficiently large 3D snapshots that, in statistical sense, correspond to the solar atmosphere.

3D R-MHD modeling

Increasingly realistic 3D R-MHD simulation of the group of Prof. Mats Carlsson (Univ. of Oslo)

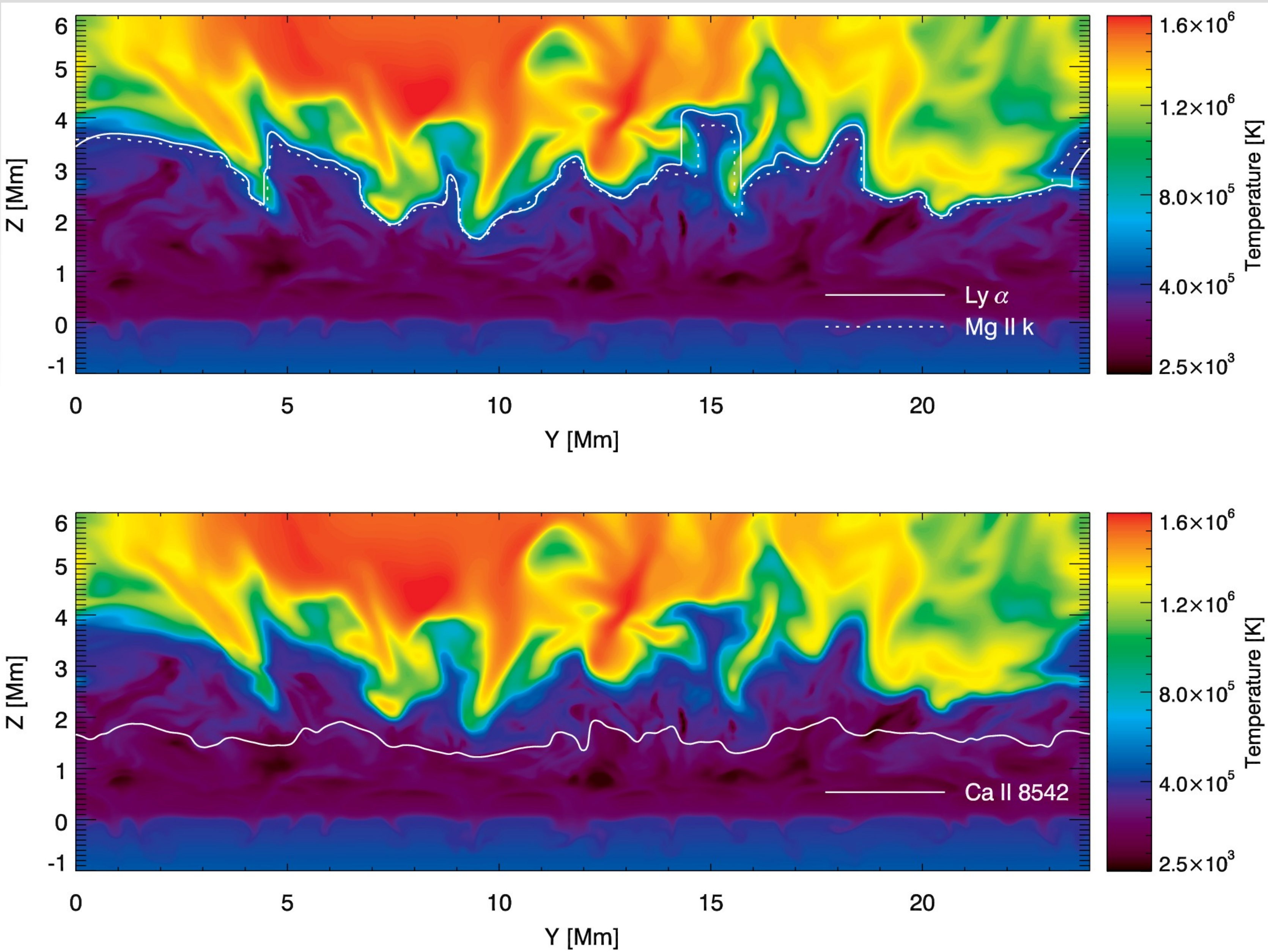
Simulation of an enhanced network region, 1 hour of real solar time.



(Leenaarts et al., 2012)

Cartesian rectilinear grid with periodic horizontal boundary conditions:
500^3 = **1.25×10^8 points** (6 orders of magnitude larger than 1D semi-empirical models)

3D R-MHD modeling



PORTA: 3D NLTE solver

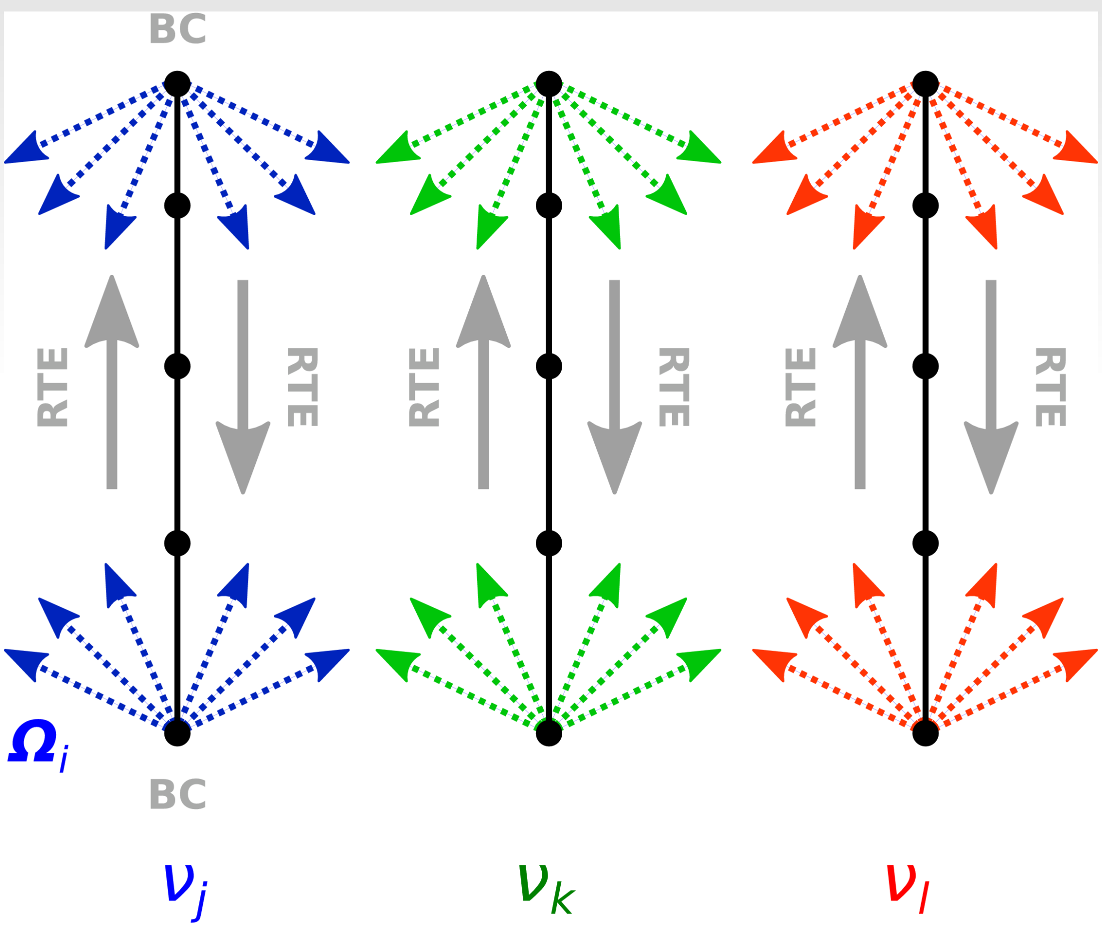
PORTA: POlarized **R**adiative **T**r**A**nsfer Solver

PORTA design goals:

- Forward non-LTE synthesis of polarized spectral lines in the full 3D geometry
- Capability to treat scattering polarization, Hanle, and Zeeman effect
- Accurate and stable formal solver of RTE
- Rapid convergence
- Massive parallelization
- Extendable modular design

Numerical NLTE

The space of the problem:



Discretization of the problem:

- Spatial grid (1D, 2D, 3D, various coordinates), ~10^2 – 10^3 points per axis
- Angular grid (~10^2 directions)
- Frequency grid (~10^3)

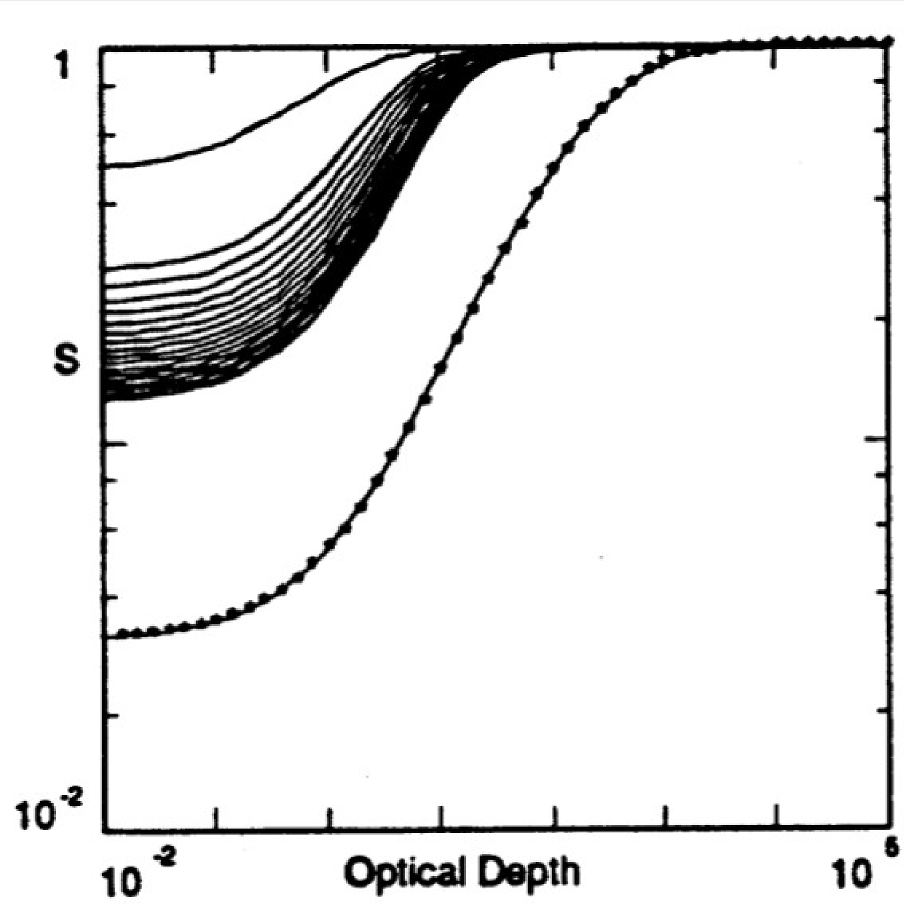
3D problem: ~10^{14} variables to process in every iteration

The goal: **self-consistent solution (ESE+RTE) density matrix elements ρ^K_Q** in all the mesh points.

Non-linear problem: Iterative solution is necessary

The convergence of the NLTE problem

Lambda iteration: Each iteration propagates the information by $\Delta\tau \approx 1$. Number of necessary iterations: **~ 1/ε** (Chromospheric lines: ε << 1)



(Auer, 1991)

Accelerating the convergence

In PORTA we use a highly convergent **multigrid method** (Fabiani Bendicho, Trujillo Bueno, & Auer, 1997) with optimal convergence behavior

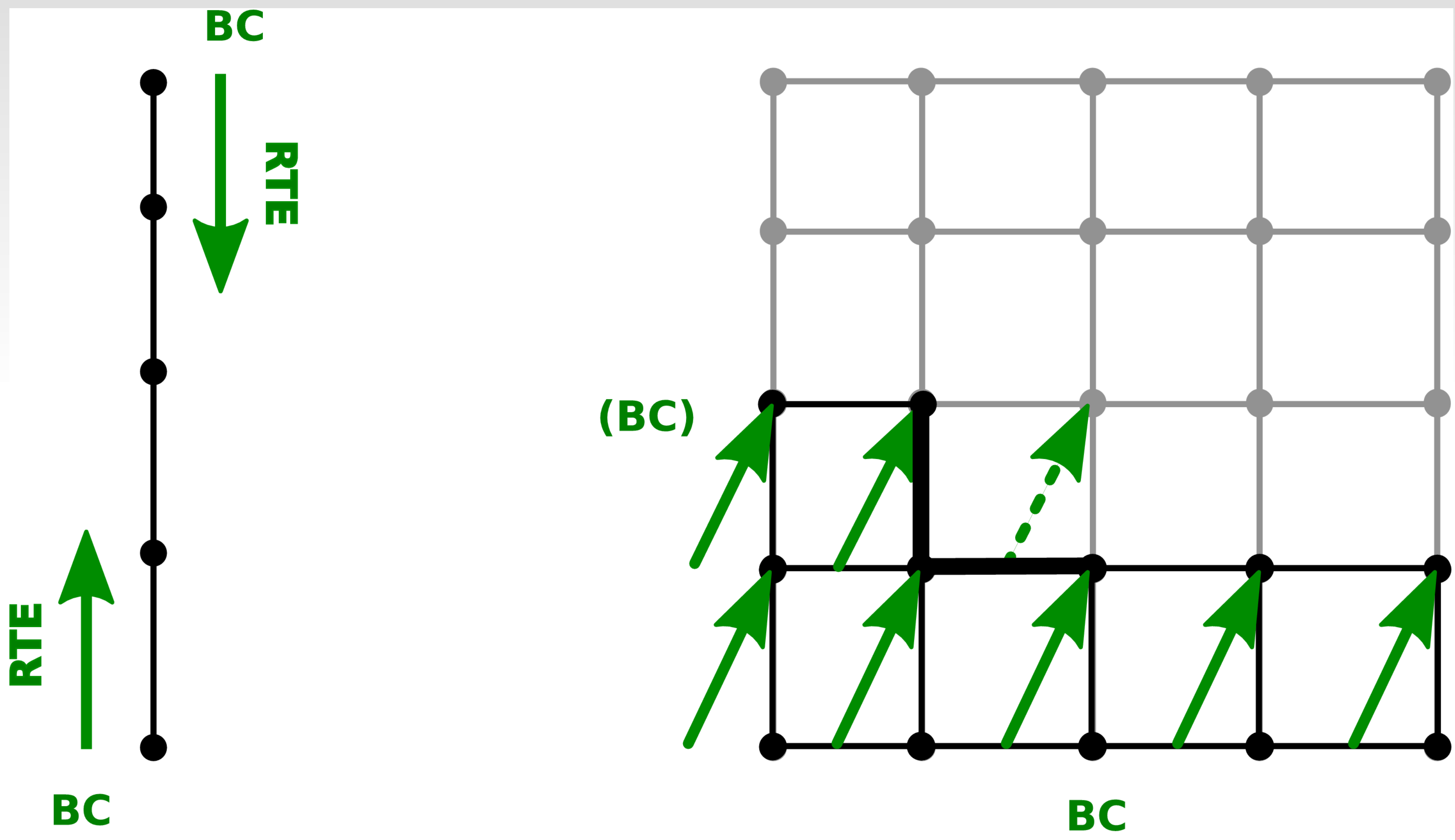
O(N), ***N*** : number of grid points

... the number of iterations does not depend on the size of the grid.

The non-LTE problem of any grid size can be solved within an effective time of 10-30 Jacobi iterations.

Formal solution of RTE using the Short Characteristics

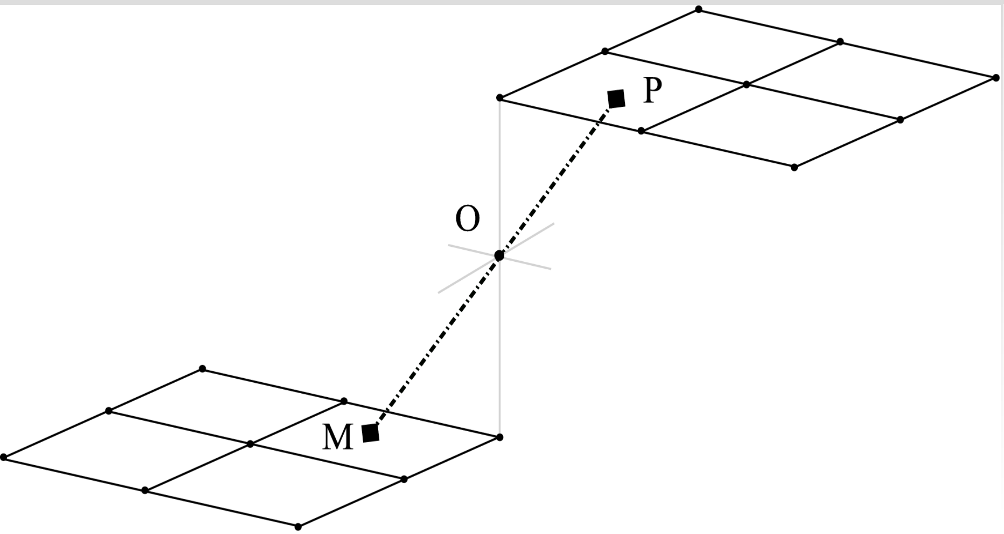
Formal solution: Requirement of a **topologically sorted mesh points**:

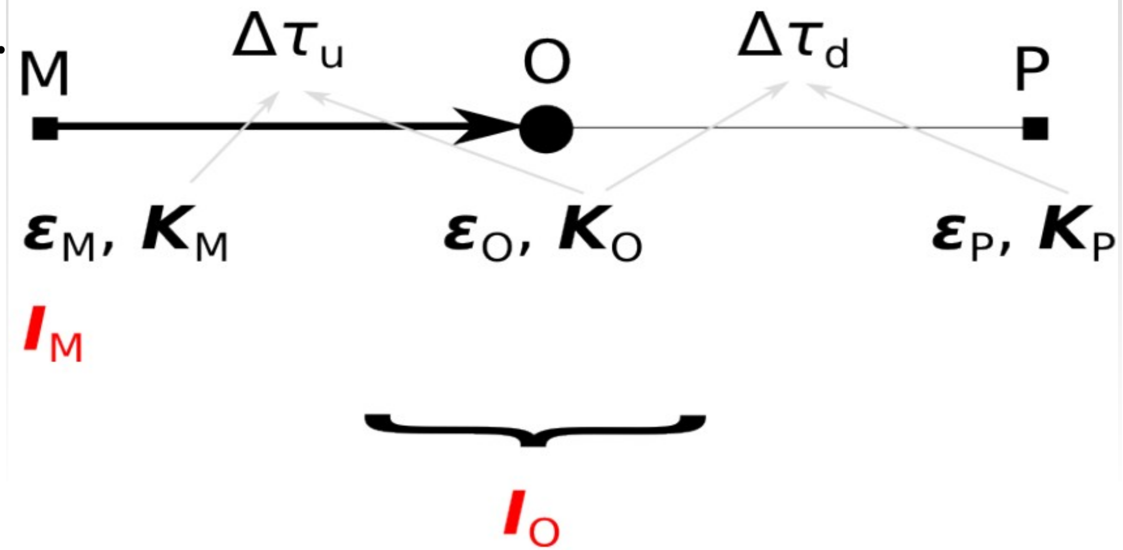


Parallelization by domain decomposition is not trivial

The method of short characteristics in detail

The short-characteristics method (Kunasz & Auer 1988):





The formal solution in the short-characteristics method:

Formally integrate

$$\boldsymbol{I}_O = \boldsymbol{I}_M e^{-\tau_{MO}} + \int_O^M \left[\frac{\boldsymbol{\epsilon}}{\eta_I} - \left(\frac{\boldsymbol{K}}{\eta_I} - \boldsymbol{1} \right) \boldsymbol{I} \right] e^{-(\tau - \tau_O)} \, d\tau$$

to obtain the Stokes parameters in O

Accuracy of solution critically depends on the interpolation method.

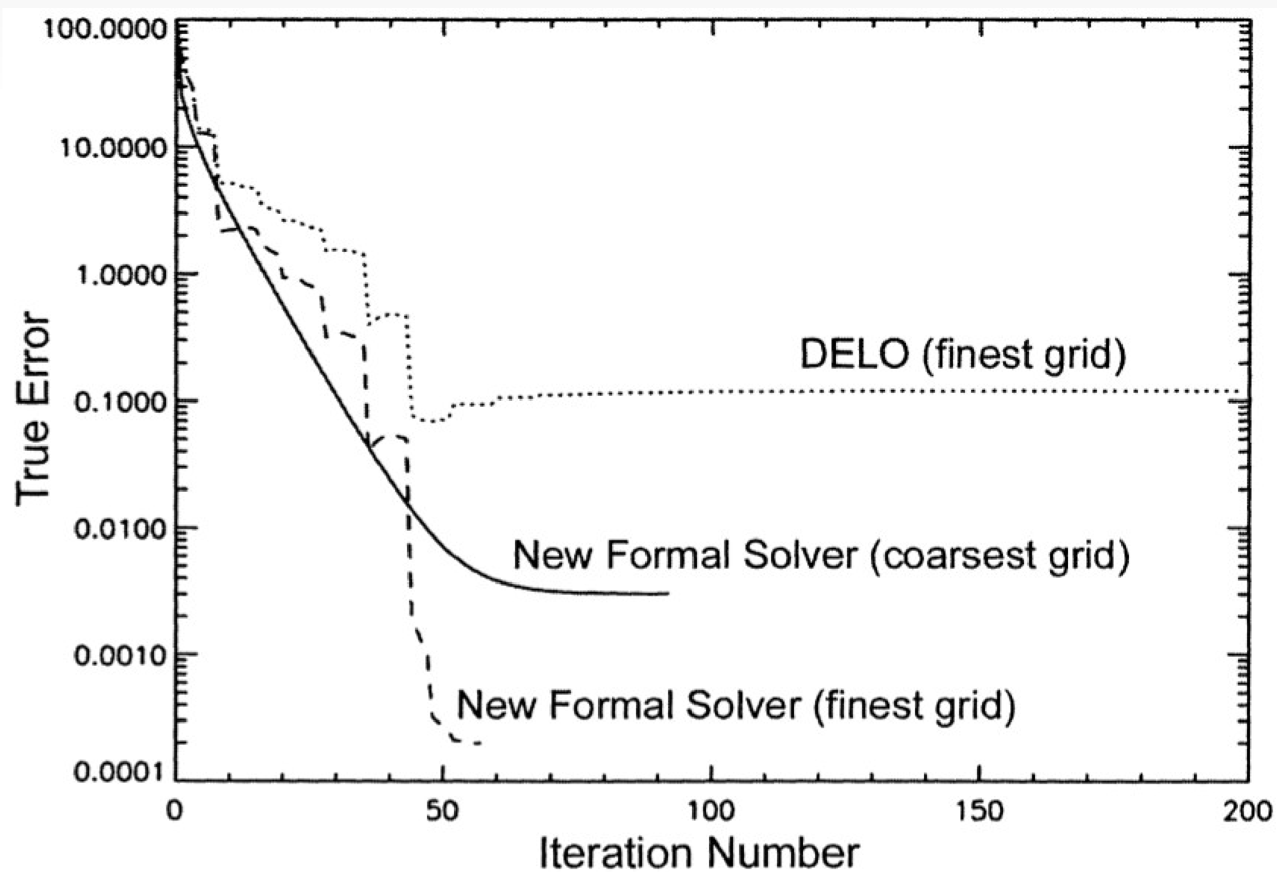
Linear interpolation

In polarized RT the **DELO** method by Rees & Murphy (1989).

Only two points MO are needed, ***S*** varies linearly with τ.

Pros: **Stable and physically consistent** (no spurious extrema)

Cons: **First-order integrator** (**error ~ Δz**) is inaccurate even in fine grids (**extremely fine grids are needed**)



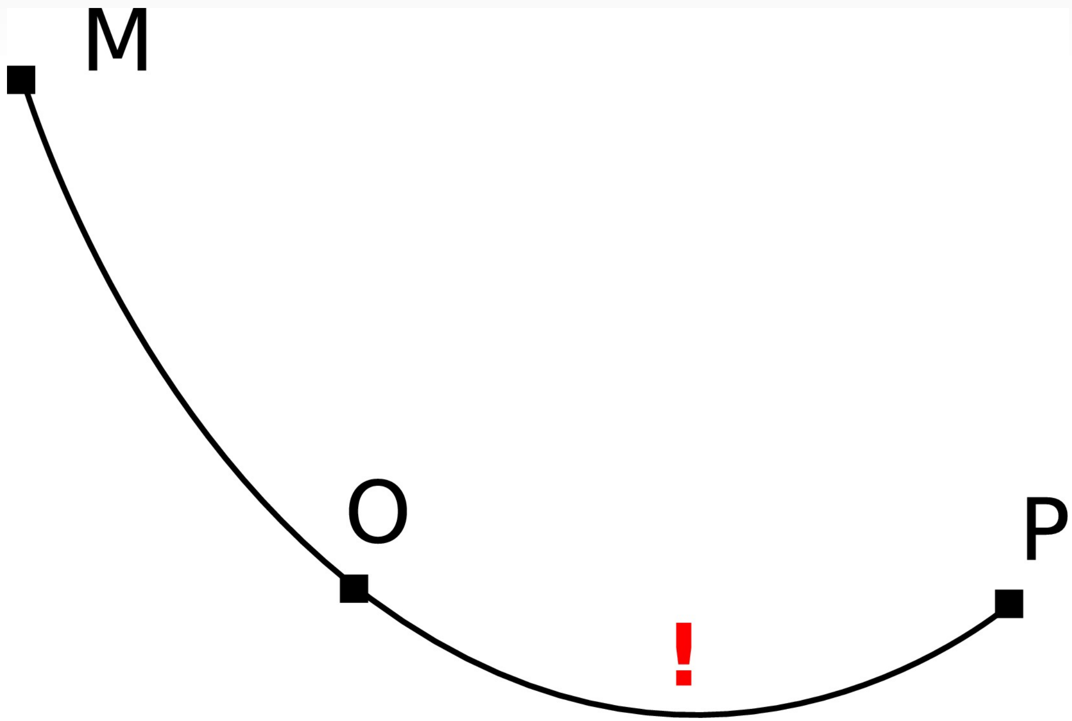
(From Trujillo Bueno 2003)

Quadratic interpolation

Parabolic interpolation in MOP: The **DELOPAR** method (Trujillo Bueno 2003).

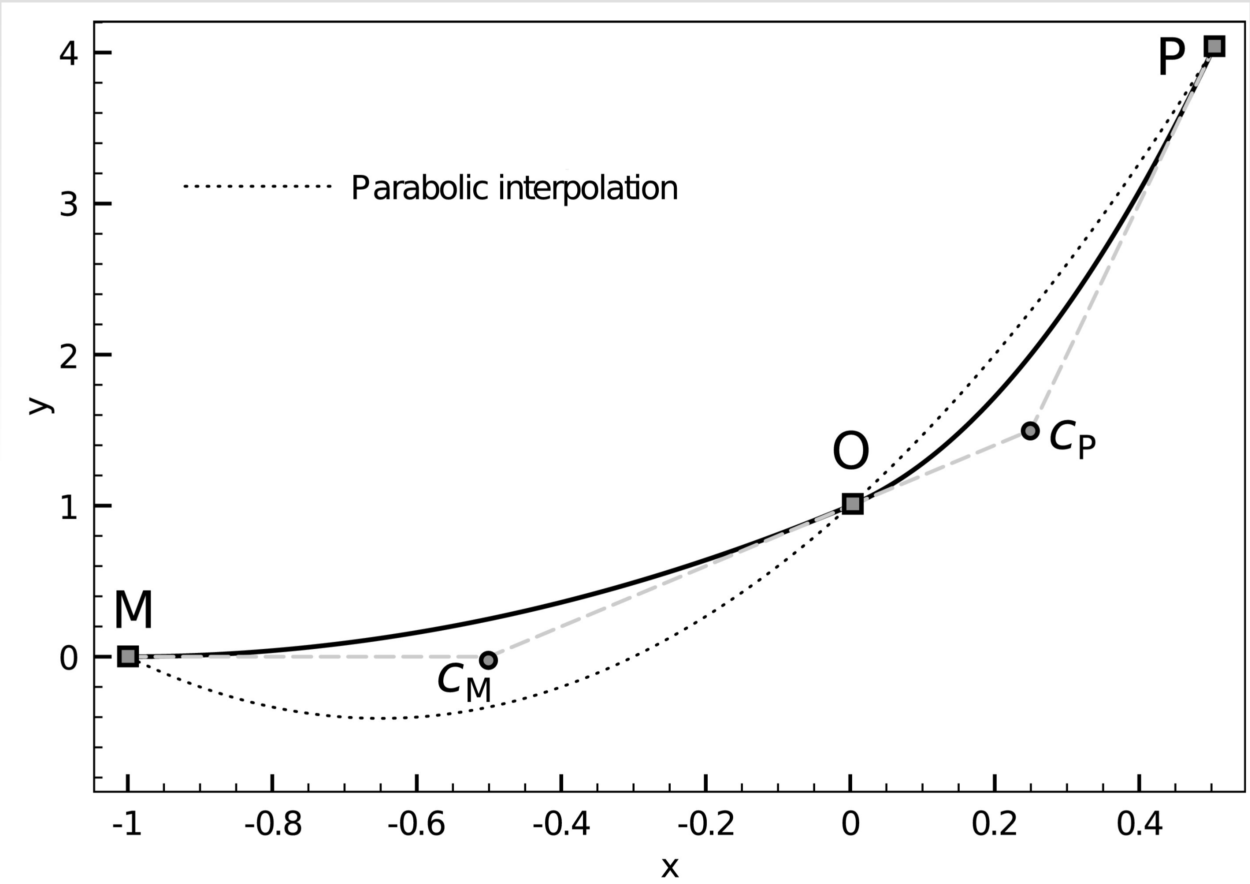
Pros: Second-order integrator (**error ~ Δz^2**), accurate in sufficiently fine grids

Cons: **Not monotonic;** Can lead to spurious extrema (overshoots) in coarse grids leading to incorrect results (negative intensities) and/or mis-convergence of the non-LTE solver (typical in the realistic MHD models). Mis-convergence in 1 point out of 100 million causes mis-convergence of the whole model!



Bezier/Hermite splines: BESSER solver

Auer (2003) suggested Bezier/Hermite splines allowing to preserve monotony.

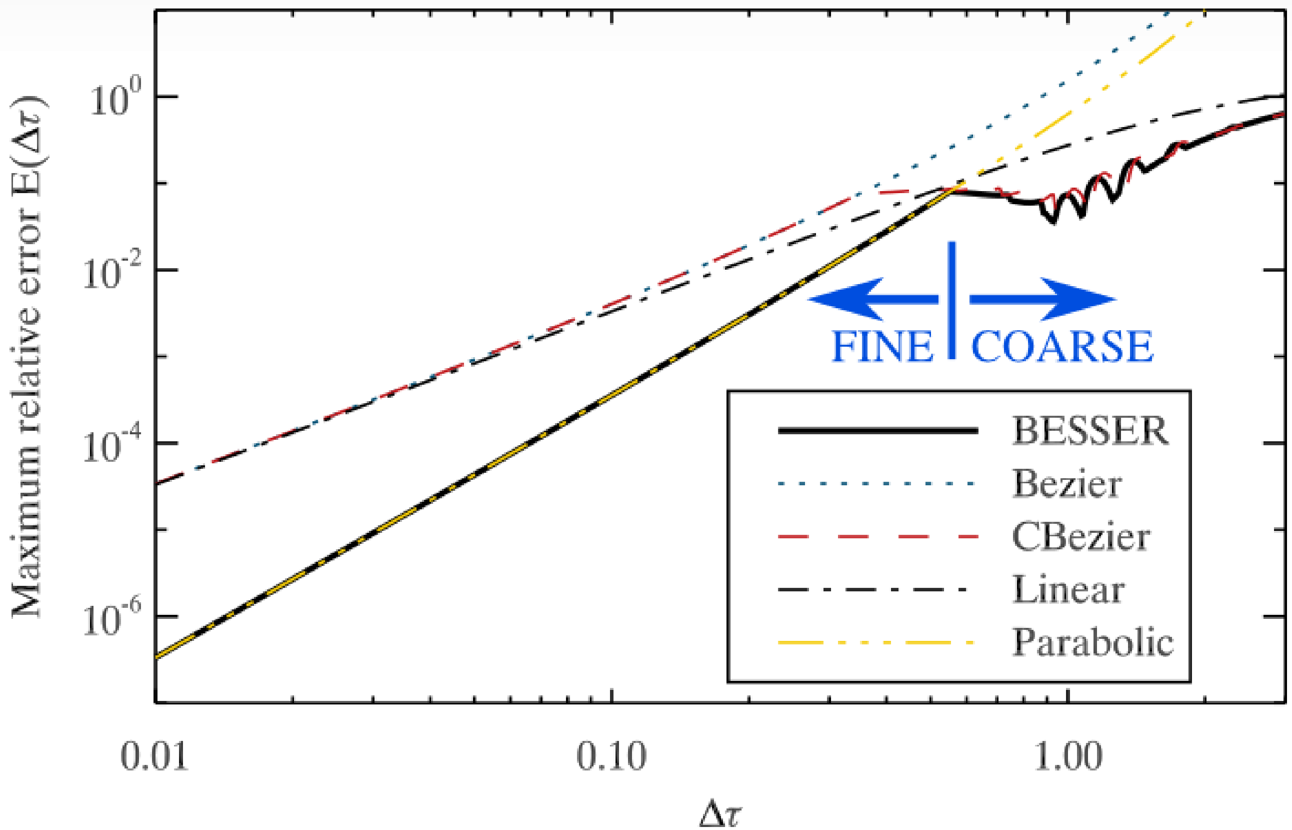


Recently several implementations for unpolarized or polarized radiation:
Hayek (2008), de la Cruz Rodriguez & Piskunov (2013), Ibgui et al. (2013), ...

A delicate problem: Most of these implementations do well reduce the spurious extrema but they **do not lead to a second-order integrator**.

Accuracy of BESSER

- Physical: no overshoots in coarse grids
- 2nd order: exactly integrates up to the 2nd order polynomials
- Stable: Λ^* in [0,1)
- Continuous 1st derivative at the central point O



Duration of the formal solution

A typical 1D model for 5-level Ca II (with sufficiently fine quadratures):
100 grid points, 1000 frequencies, 100 ray directions, 4 Stokes parameters.

With nowadays CPUs: 1 grid point + 1 frequency + 1 direction + 1 Stokes ~ **10^{-6} s**

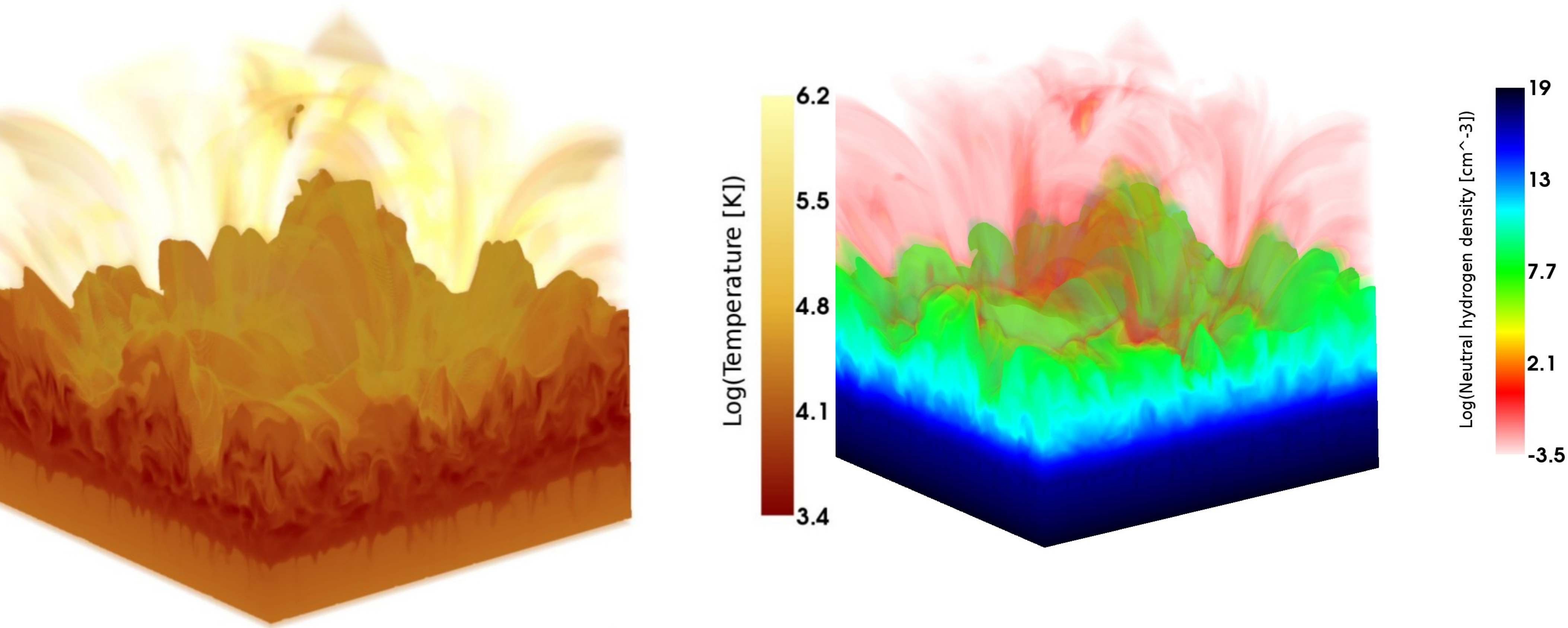
One formal solution duration = $100 \times 1000 \times 100 \times 4 \times 10^{-6}$ = **40 s**

Full convergence (~20 iterations) **~ 13 minutes**.

Memory requirements ~ **50 kB**

Formal solution in 3D

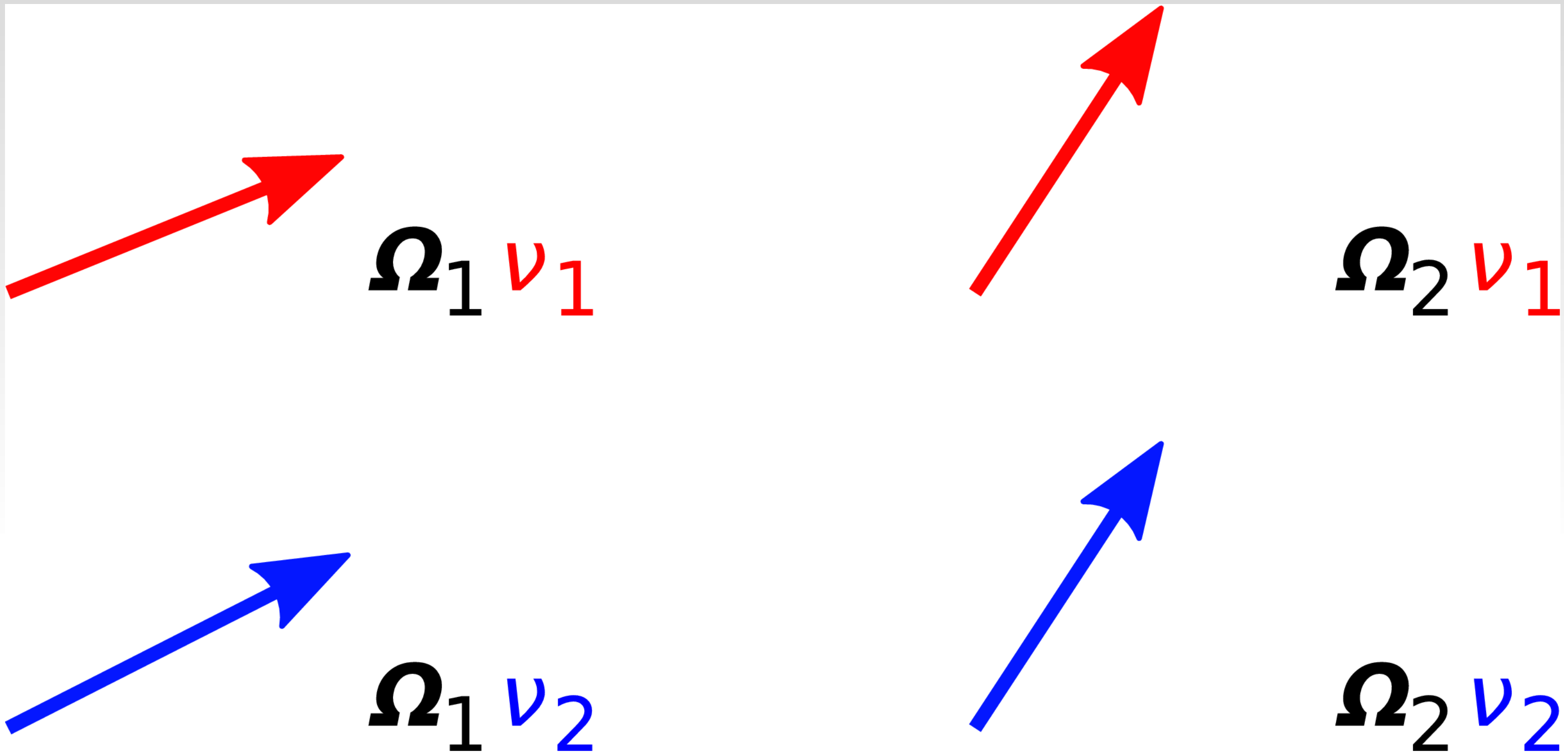
A practical example of a 3D snapshot of an MHD simulation:



500^3 = **125 x 10^6 points** (6 orders of magnitude larger than 1D semi-empirical model)

Formal solution duration: **580 days (parallelization of FS is necessary)**
Memory requirements: **60 GB (domain decomposition is necessary)**

Formal solution in using serial solver



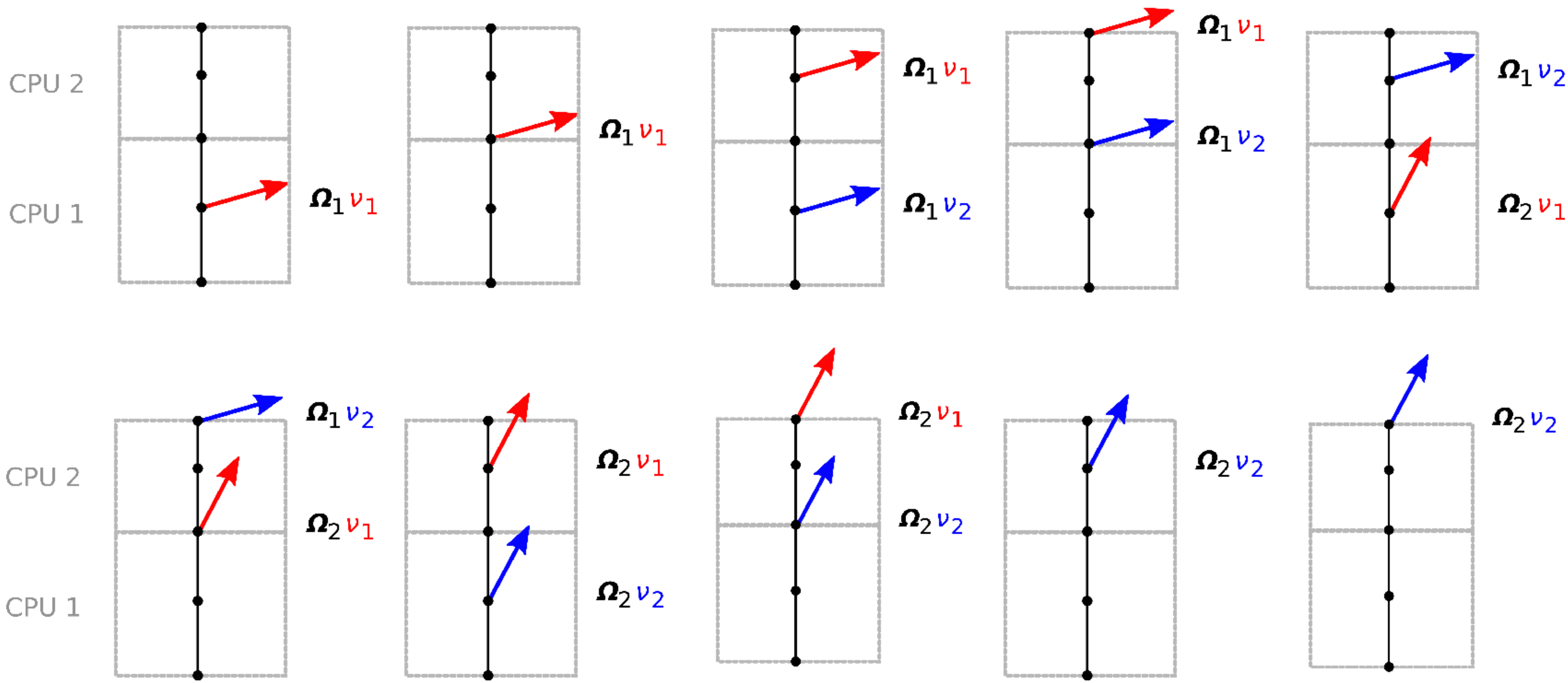
Serial solution: 1 grid point, 1 direction, 1 frequency at 1 time step

Duration of calculation is proportional to $N_{\text{grid points}} \times N_{\Omega} \times N_{\nu}$

Directions X Space parallelization

Decompose the grid into **horizontal domains** (slabs), each treated by one CPU.

Process the **Directions X Frequency** discrete space in a synchronized way



Acceleration: 10 time steps instead of 16

Directions X Space X Frequency parallelization

Additional "orthogonal" parallelization:
Each CPU can treat only a limited number of frequencies:

L : number of domains (slabs)
M : number of frequency intervals per processor
N_Ω : total number of short-characteristics directions
N_ν : total number of radiation frequencies

Speedup S of the solution with respect to the serial solution:

$$S(ML) = ML\frac{1}{1+\lambda}, \qquad \lambda = \frac{2M(L-1)}{N_\Omega N_\nu}$$

Example (10,000 CPUs):

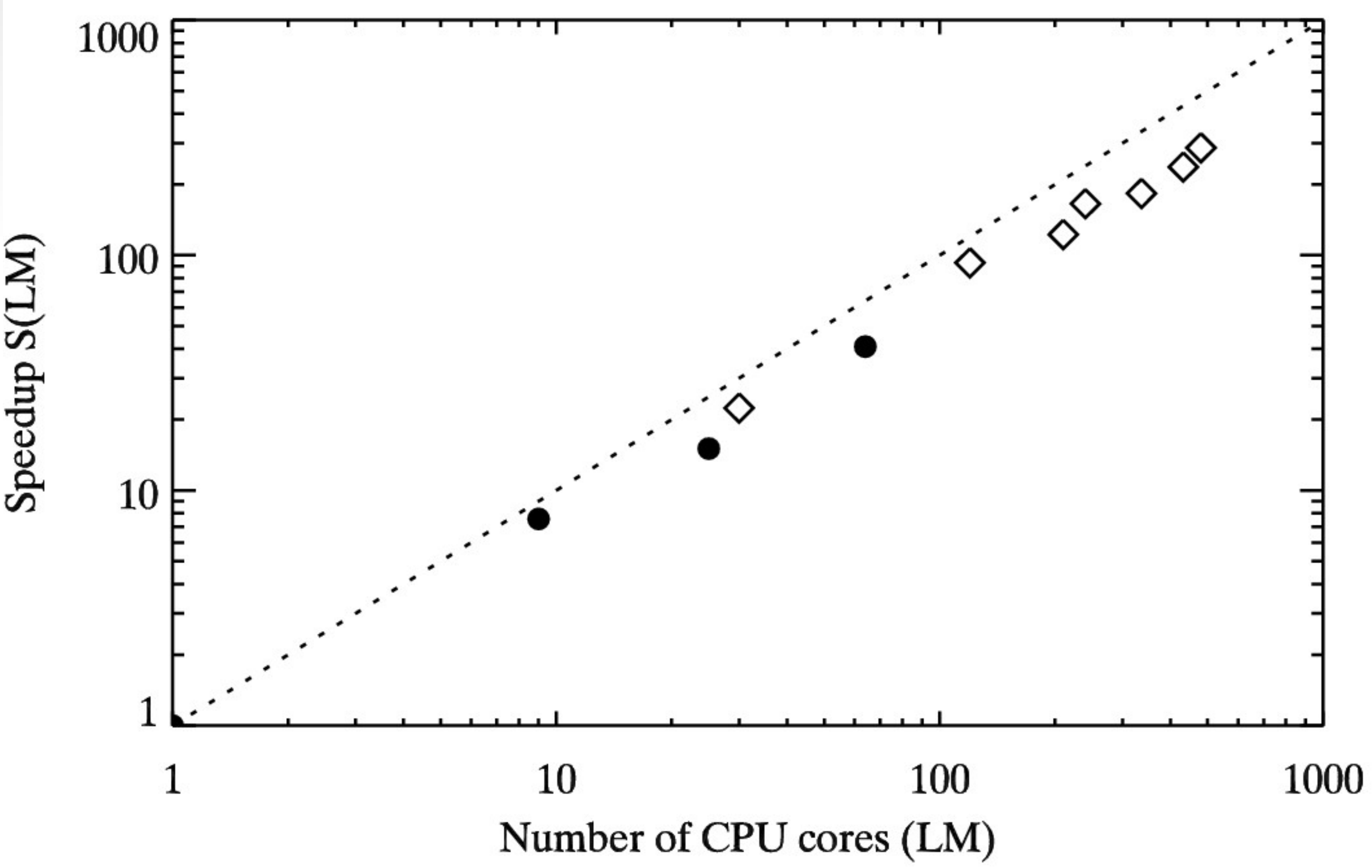
$L = 100$
$M = 100$
$N_\Omega = 100$
$N_\nu = 1000$

$\boldsymbol{\lambda = 0.2}$
S(10,000) = 8400

Scaling of the SA

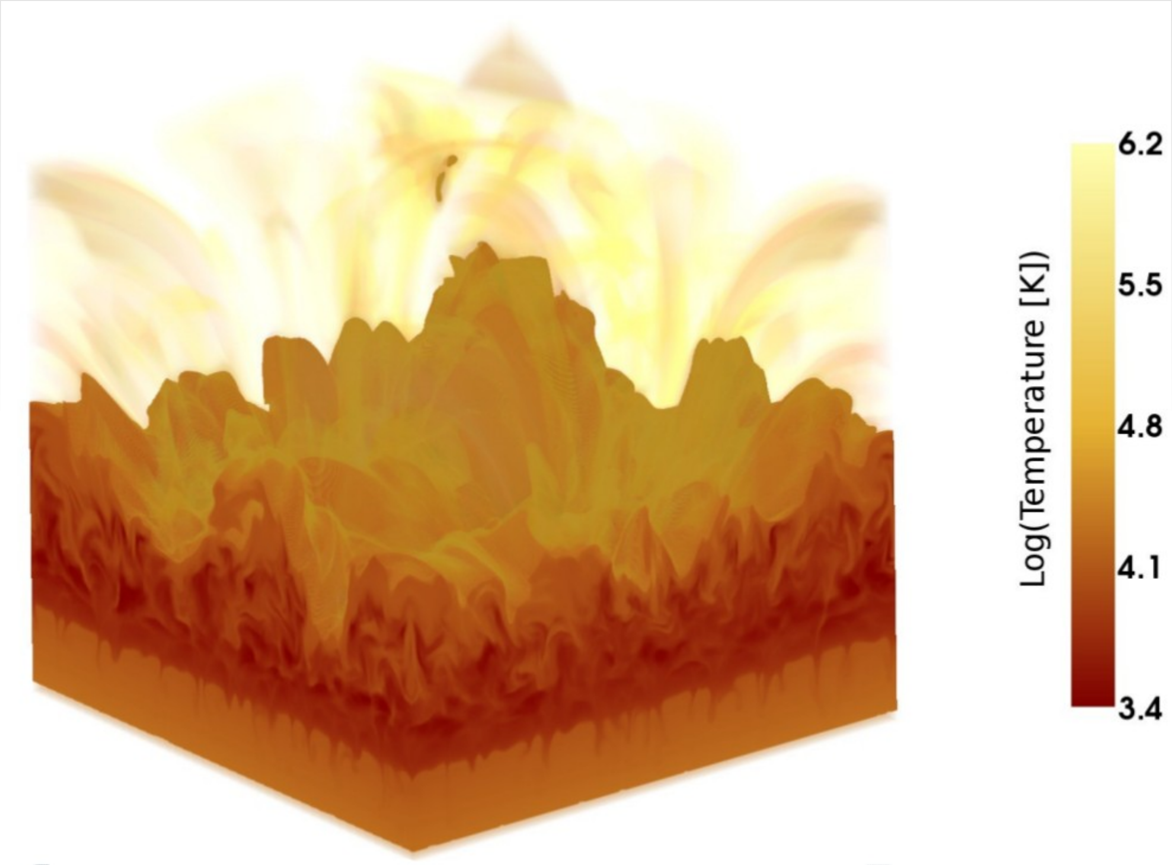
Numerical benchmarking for 3D models of **5-level Ca II** and **Lyman-α** at **Ondřejov cluster**, **LaPalma supercomputer** and the **MareNostrum** (Barcelona) supercomputer (benchmarking up to 2048 CPU cores).

MareNostrum, Barcelona
>40,000 CPUs



In practice (taking into account all MPI communication trade-of) speedup: $S \sim P^{0.9}$

Realistic application



Our previous 3D problem:

500^3 = **125 x 10^6 points**

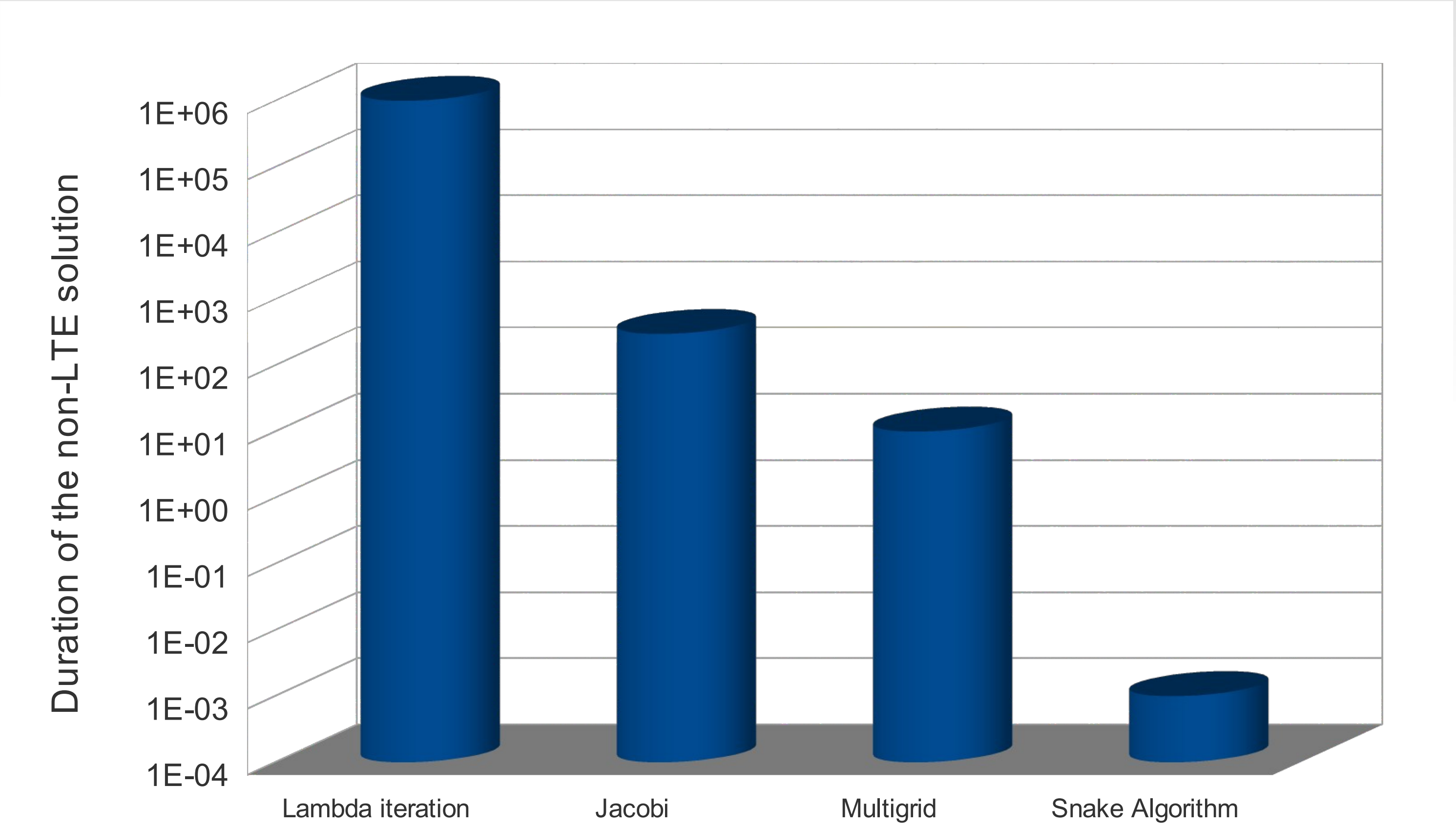
Serial formal solution: **580 days**
Full convergence: **32 years**

With 2000 CPU cores: **15 hours**
Full convergence: **12 days**

No memory problems with existing 3D models.

From Lambda iteration to parallelism

Consider a two-level non-LTE problem with $\boldsymbol{\varepsilon} = \mathbf{10^{-6}}$

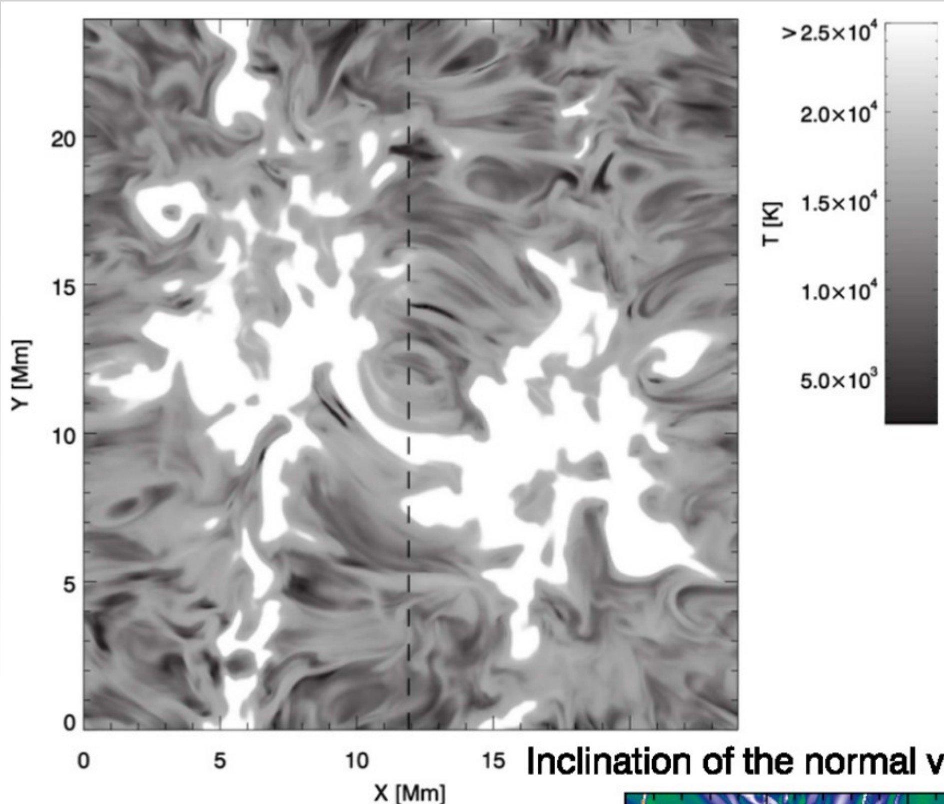


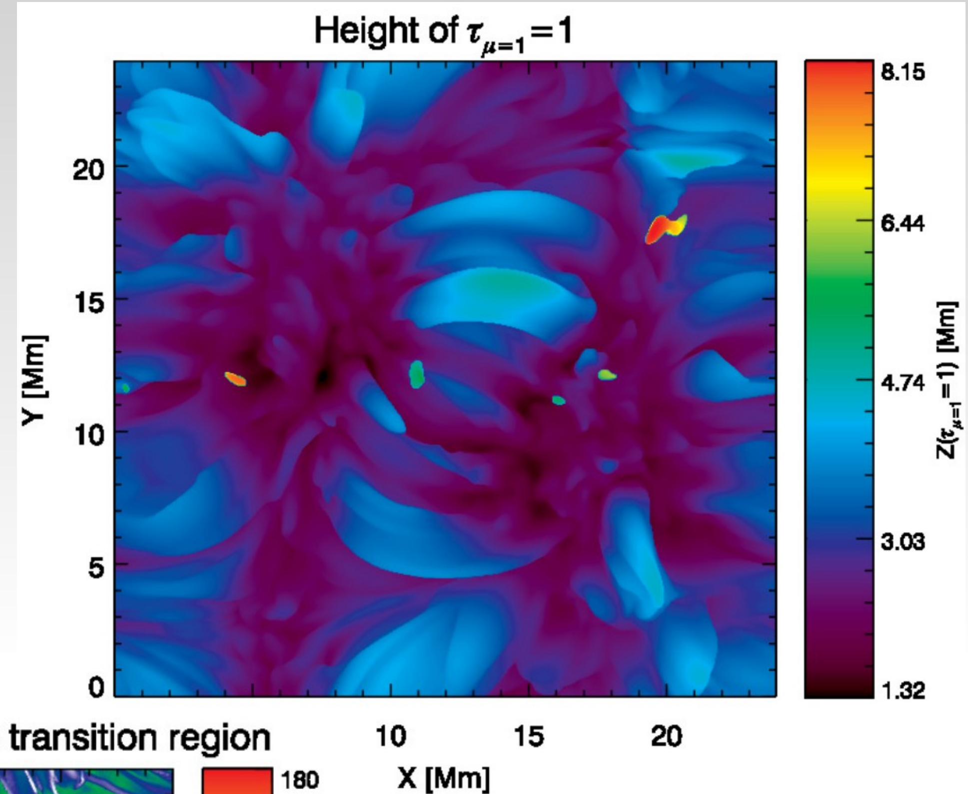
From classical Lambda iteration to parallel multigrid: Speed up by 9 orders of magnitude.

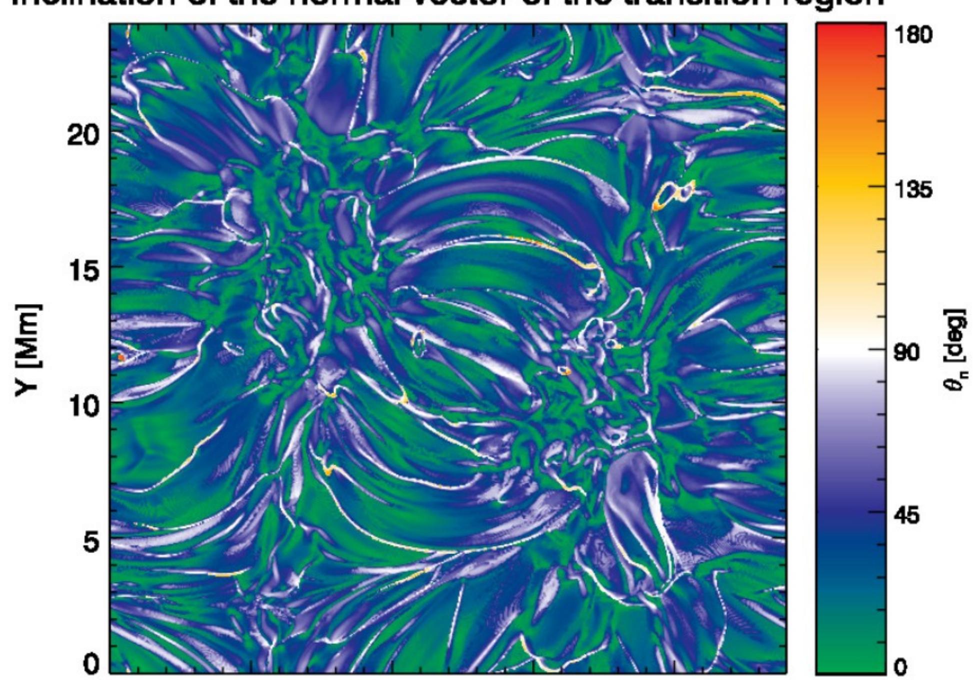
Advantages of the parallelization strategy

- Accuracy is identical to the serial solution
- The total number of FS is identical to the serial solution
- No discontinuities of errors at the domain boundaries
- Easy to save & load a partially converged solutions
- Scales almost linearly with P
- Thanks to orthogonality of the parallelizations it is suitable for massively parallel computers ($P \geq 10^4$)
- Relatively easy to implement into existing serial codes

Formation of the hydrogen Ly-α



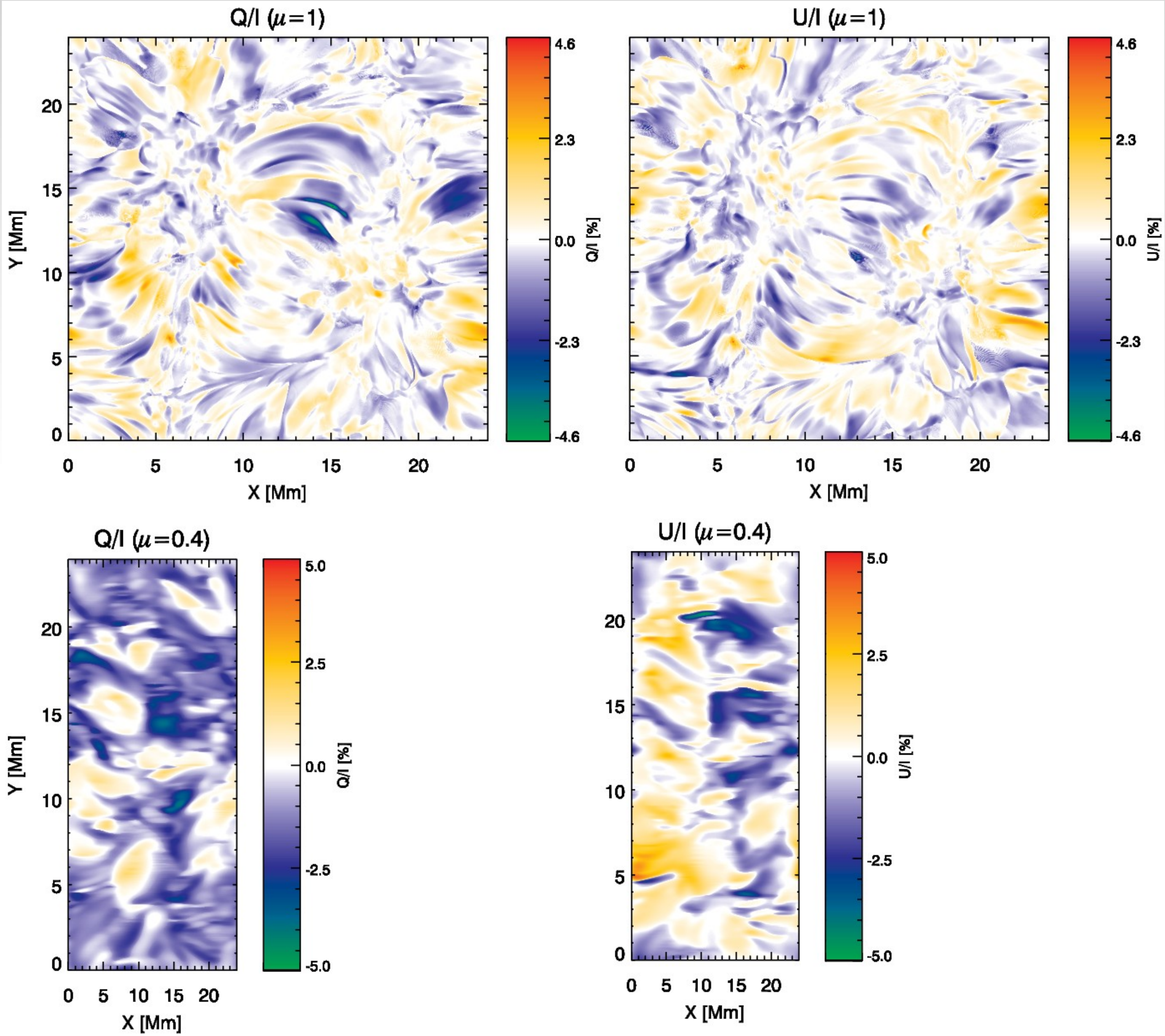




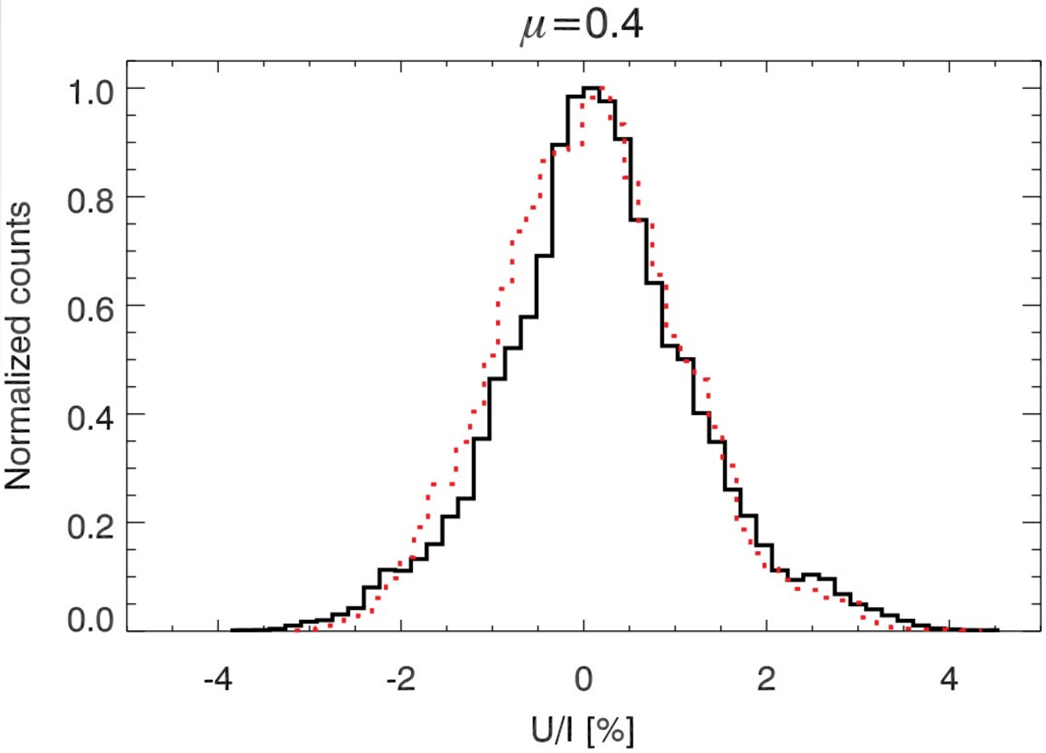
Emergent line-center polarization

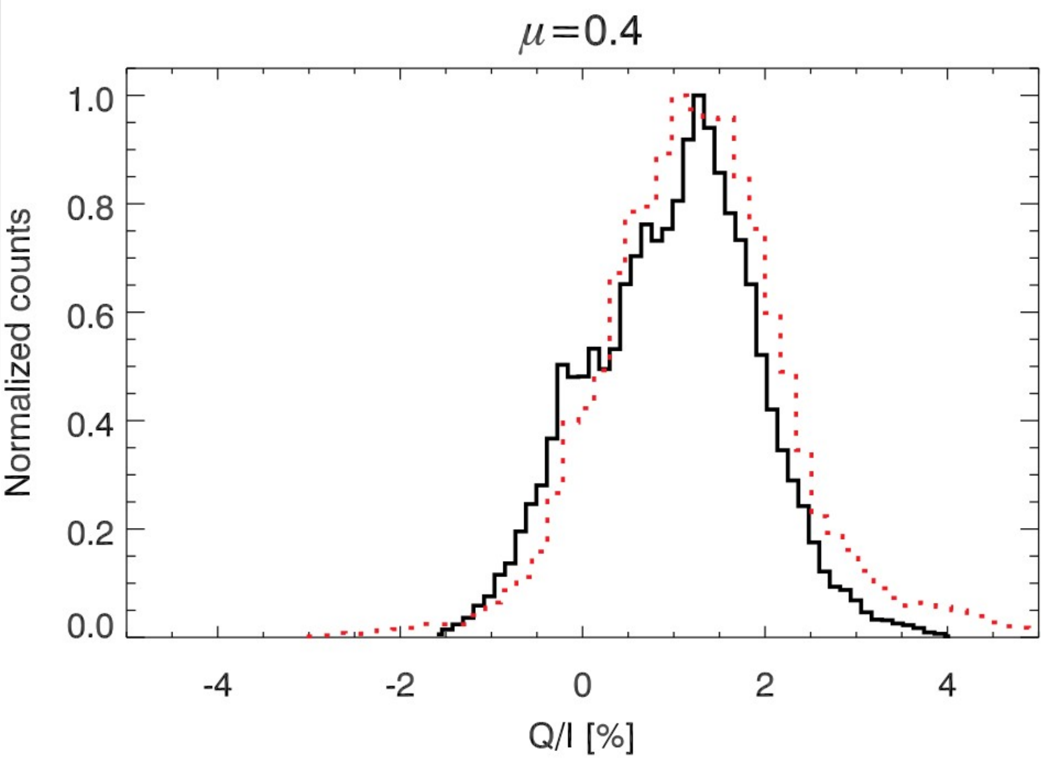
$\mu = 1$

$\mu = 0.4$

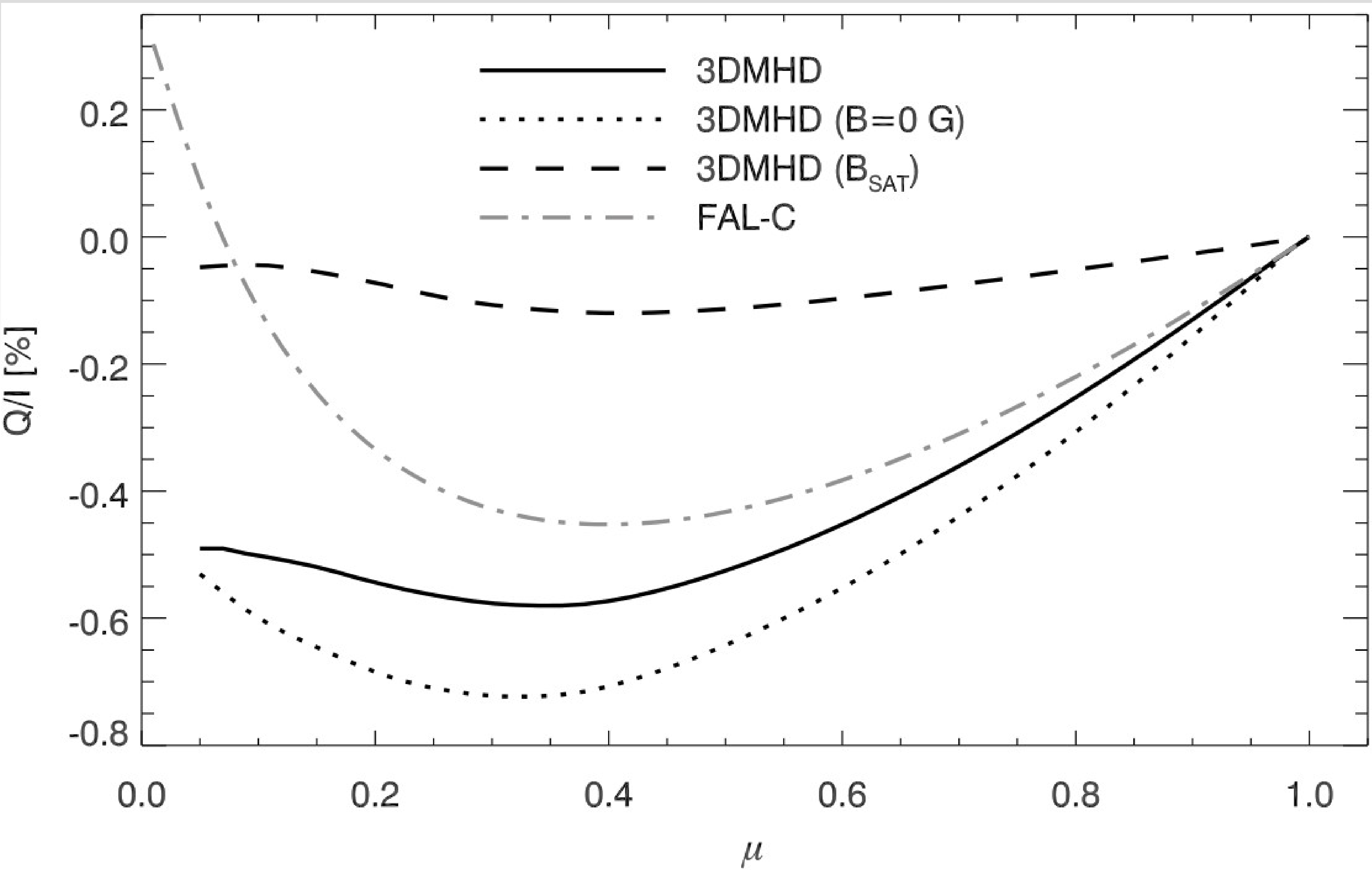


U/I and Q/I histograms at $\mu = 0.4$





Center-to-limb variation



Conclusions

- 1D still useful for several lines: good for approximate magnitude of average mg. fields
- 3D models: increasingly realistic
- Inference of average properties of the quiet atmosphere
- 3D necessary for localized structures (prominences, flares)
- Inference of the spatially resolved magnetic field?

PORTA:

First 3D multilevel polarized code for NLTE synthesis	Accurate and stable formal solver
Massively parallel	Extendable by modules: Various physical approximations can be implemented

For more information see Štěpán & Trujillo Bueno (2013), A&A 557, 143