The 3D model atmosphere code CO^{5}BOLD: methodology and tales of application

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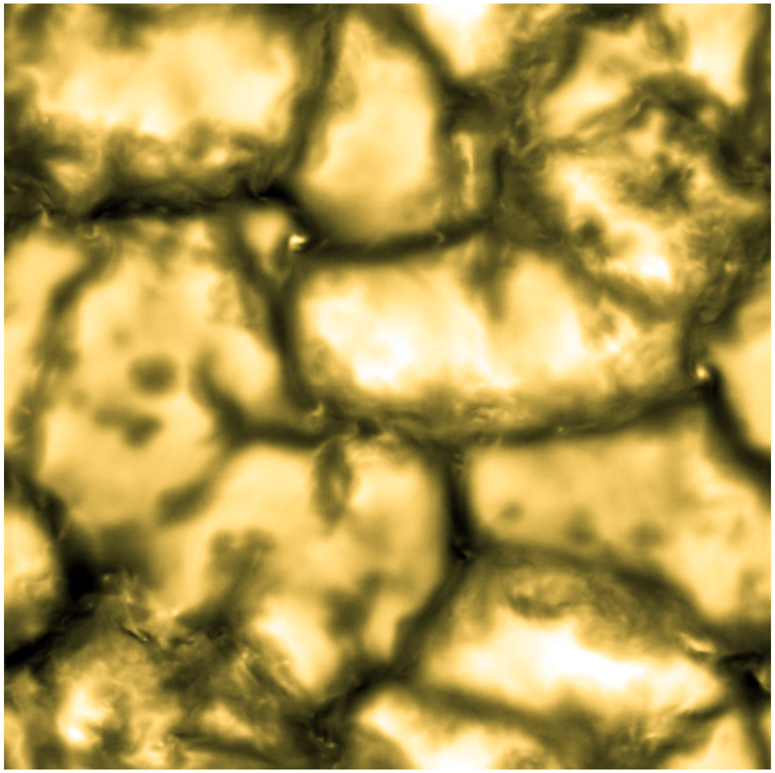
Overview

- Motivation
- CO^{5}BOLD radiation-magnetohydrodynamics code
  - HRD coverage
  - some words on 3D spectral synthesis
  - bottle-necks and places of active development
- Applications
  - solar photospheric abundances
  - (^{6}Li in the early Universe)
- Leaving out applications related to ...
  - convection properties relevant for stellar structure
  - time-dependence, turbulence $\rightarrow$ mode excitation, asteroseismology

Are stellar atmospheres horizontally homogeneous and static?



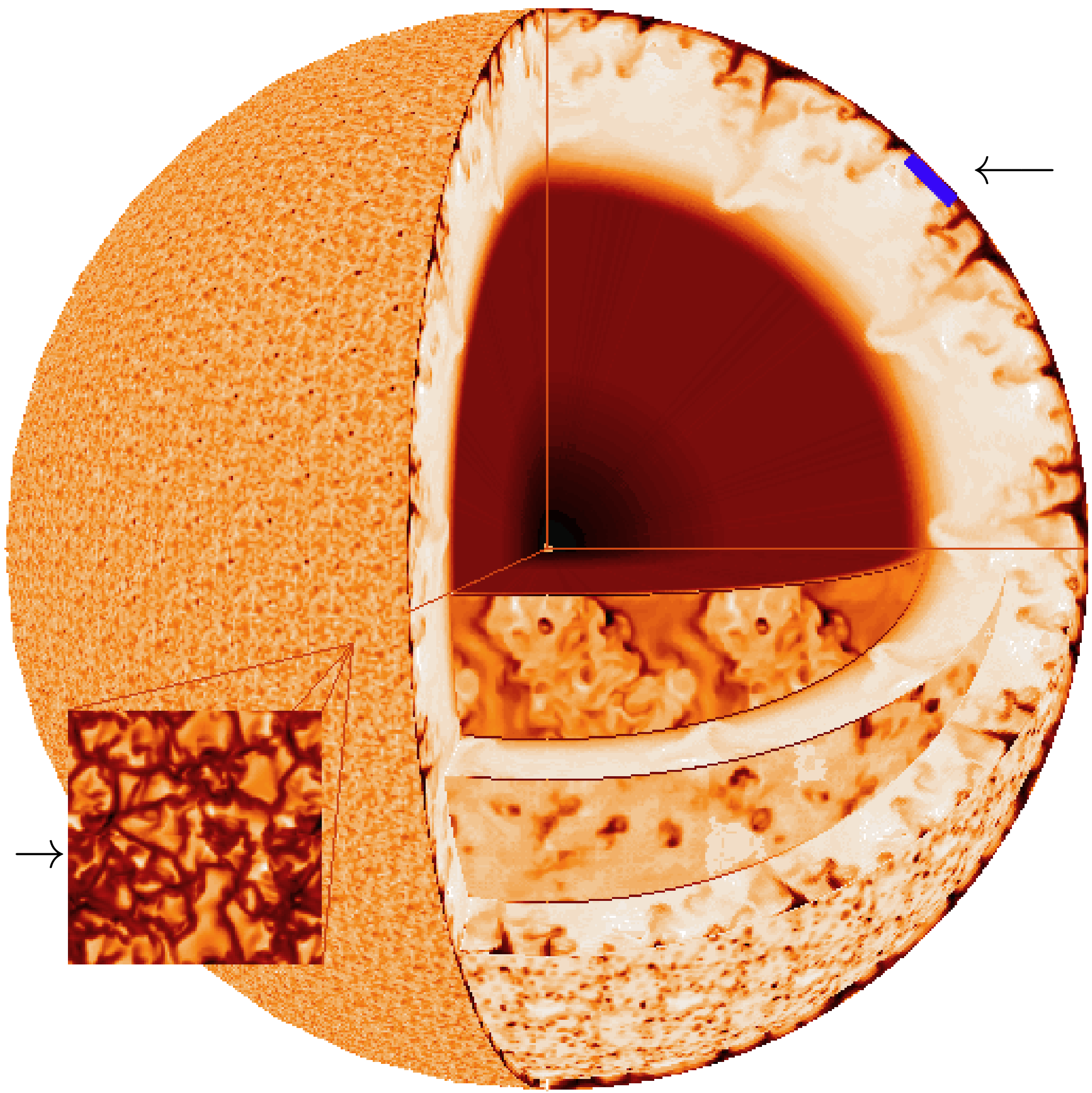
hires image of solar surface

1D model representation

- Sun as typical star with outer convective envelope: horizontal T-inhomogeneities of $\Delta T \approx 1000\,\mathrm{K}$ evolving on time scales of minutes

- How accurate are predictions of stellar properties based on 1D models?
  $\rightarrow$ abundances

Scale separation in cool stars → “box-in-a-star” setup



Solar granulation →

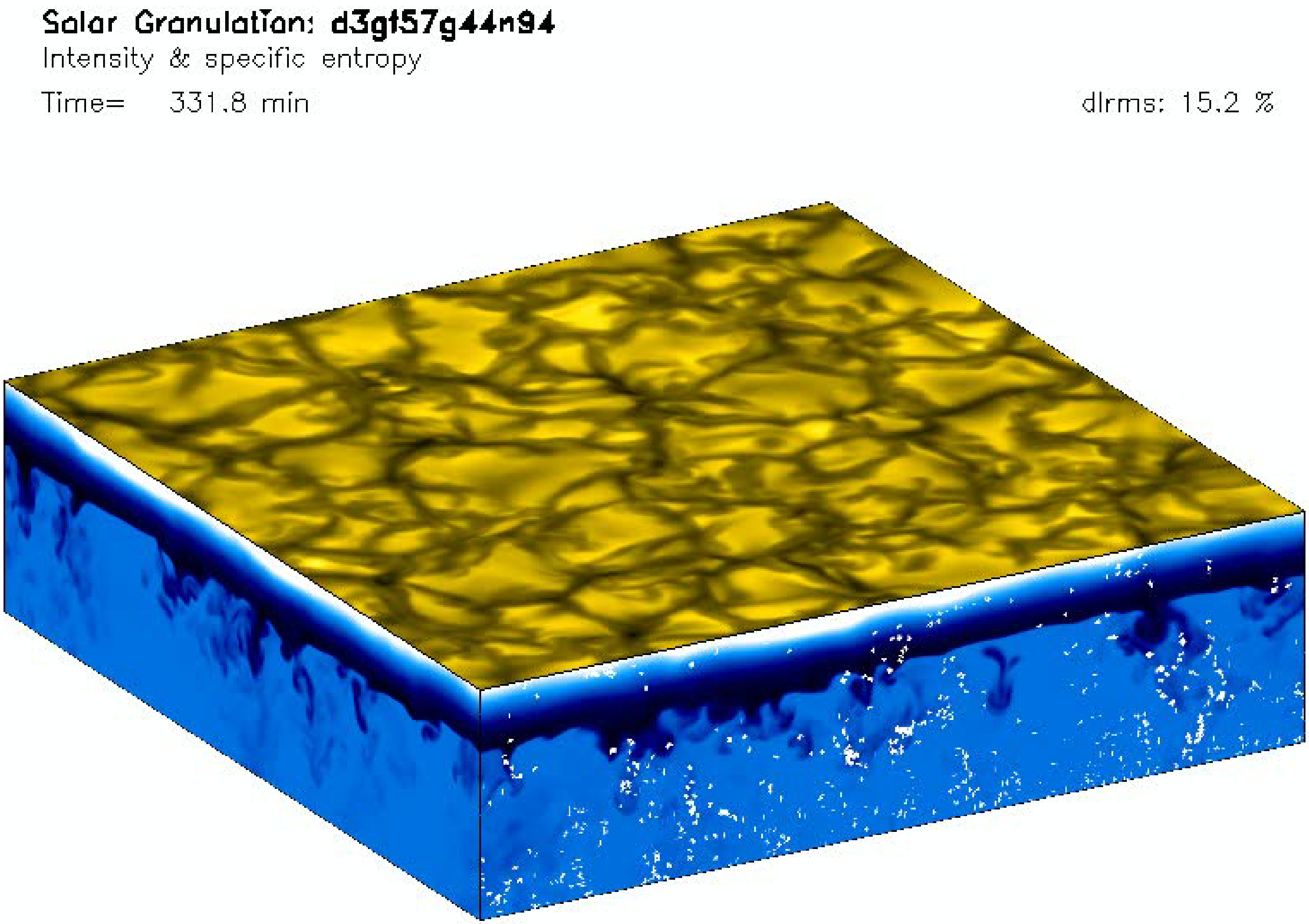
← Cartesian simulation box with periodic side boundaries

Artwork © Å. Nordlund 1995

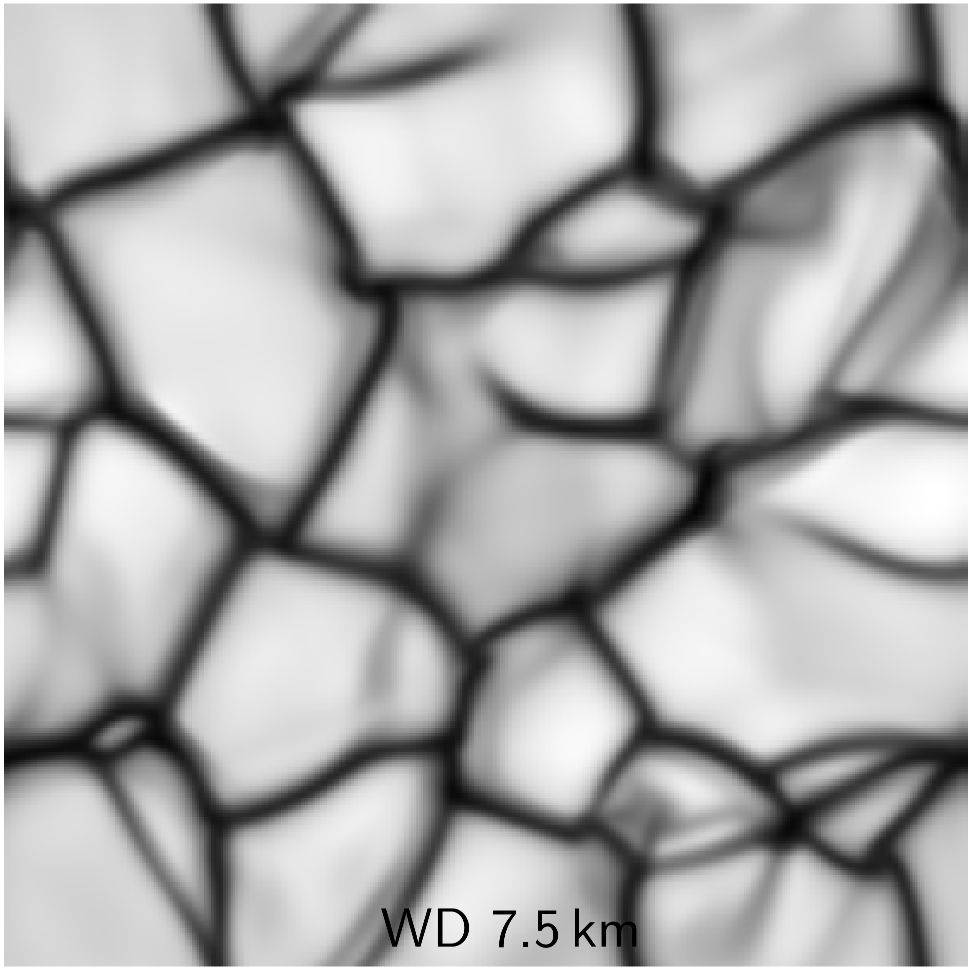
The radiation-magnetohydrodynamics code CO^{5}BOLD

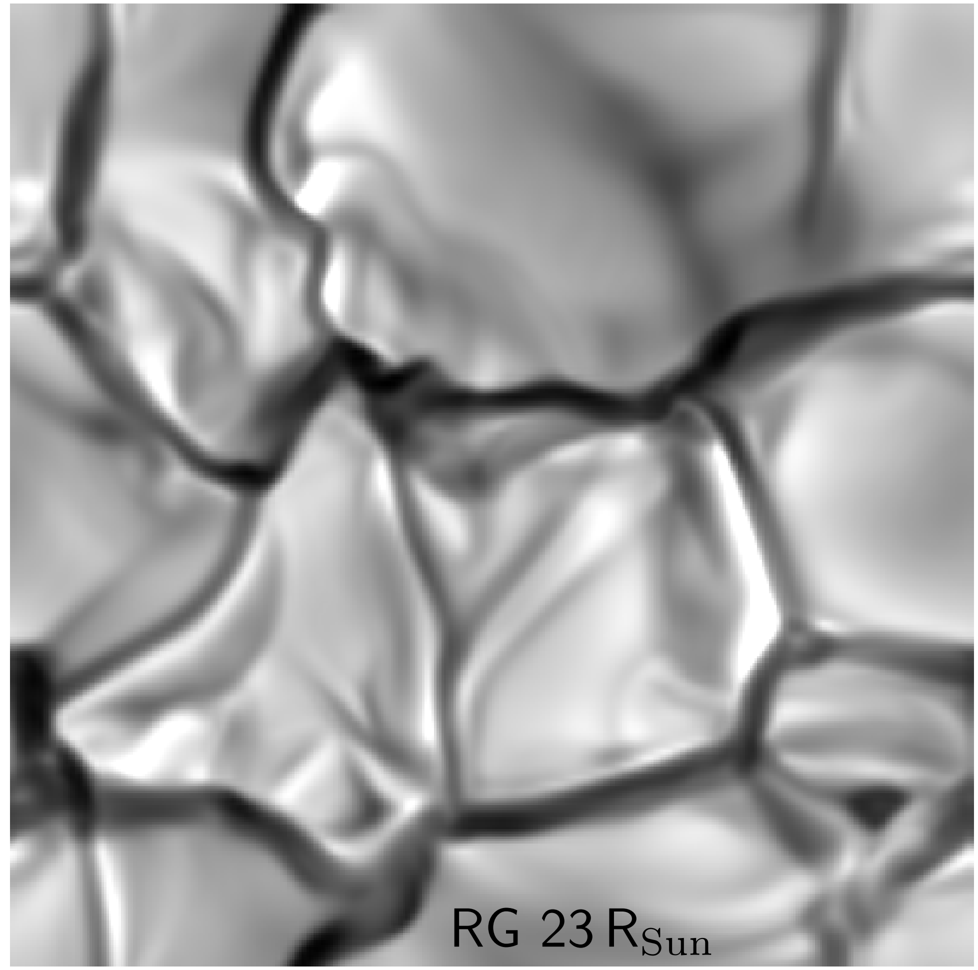
- COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with l=2,3
- B. Freytag & M. Steffen, with contributions from S. Wedemeyer, W. Schaffenberger, HGL
- Solution of the HD or MHD equations coupled to equation of radiative transfer
  - HD/MHD, approximate Riemann solvers $\rightarrow$ low intrinsic dissipation, "shock-proof"
  - wavelength dependence of radiation field treated by multi-group approach
  - realistic equation-of-state (tables)
- Kinetics & transport for molecules and dust grains, non-equilibrium chemistry
- Strictly conservative in mass, momentum, and energy
- Open top (waves) and bottom (convection) boundaries
- CO^{5}BOLD not limited to local models "box-in-a-star" $\rightarrow$ "star-in-a-box"
- Result: statistical realization of flow from sub-photosphere to chromosphere

Schematic close-up of 3D model



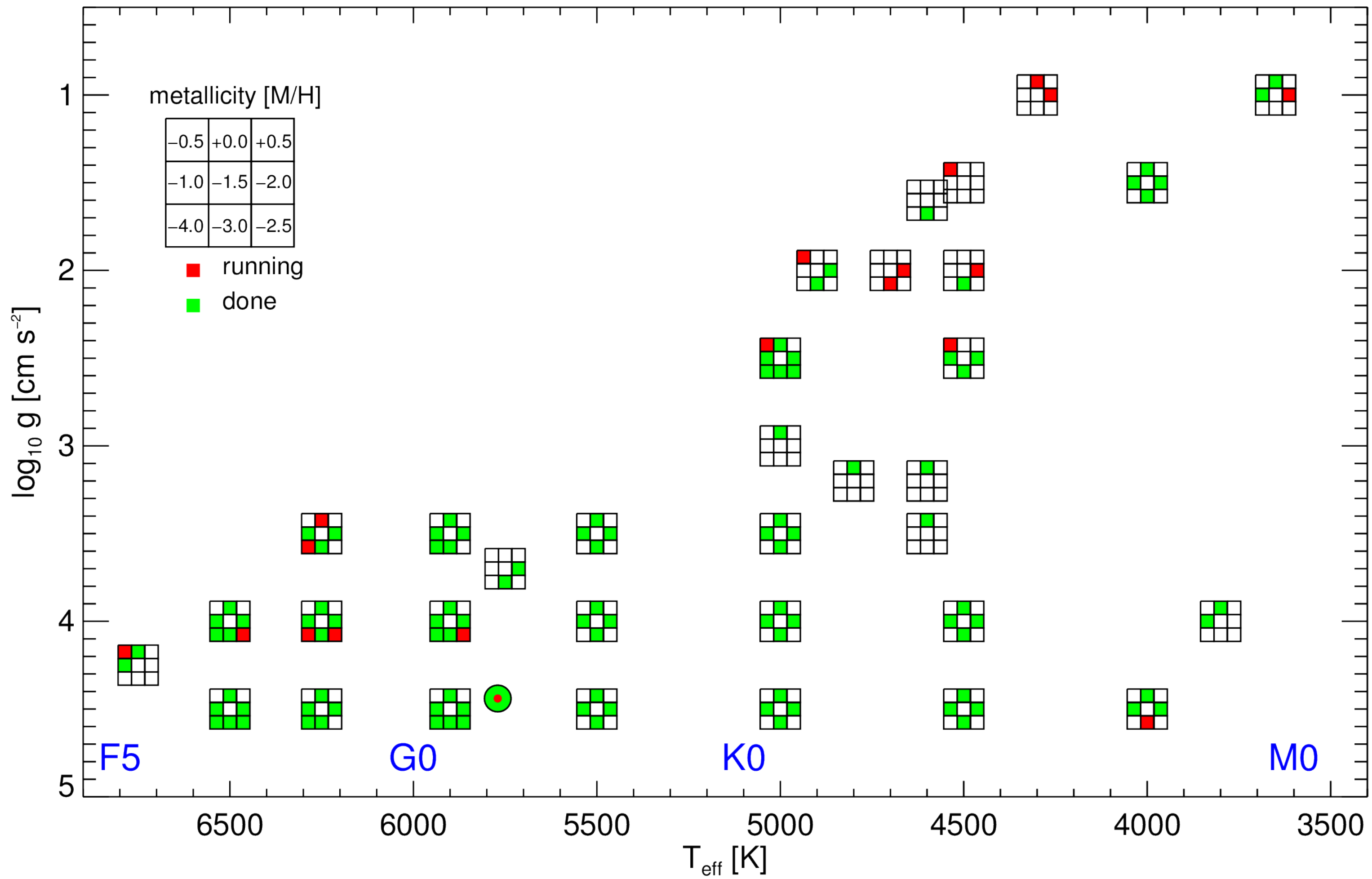
Granulation across the Hertzsprung-Russell diagram





- From the Sun to stars with largely different parameters $\rightarrow$ robustness
- Here: spatial scale ratio 2×10^6

CIFIST+ 3D model atmosphere grid of non-degenerate objects



(Ludwig, Caffau, Steffen, Freytag, Bonifacio, Kučinskas)

- Filling of parameter space mostly project driven
- In addition: M-dwarfs, AGB giants, brown dwarfs, white dwarfs . . .

Hydrogen-rich (DA) cool white dwarfs

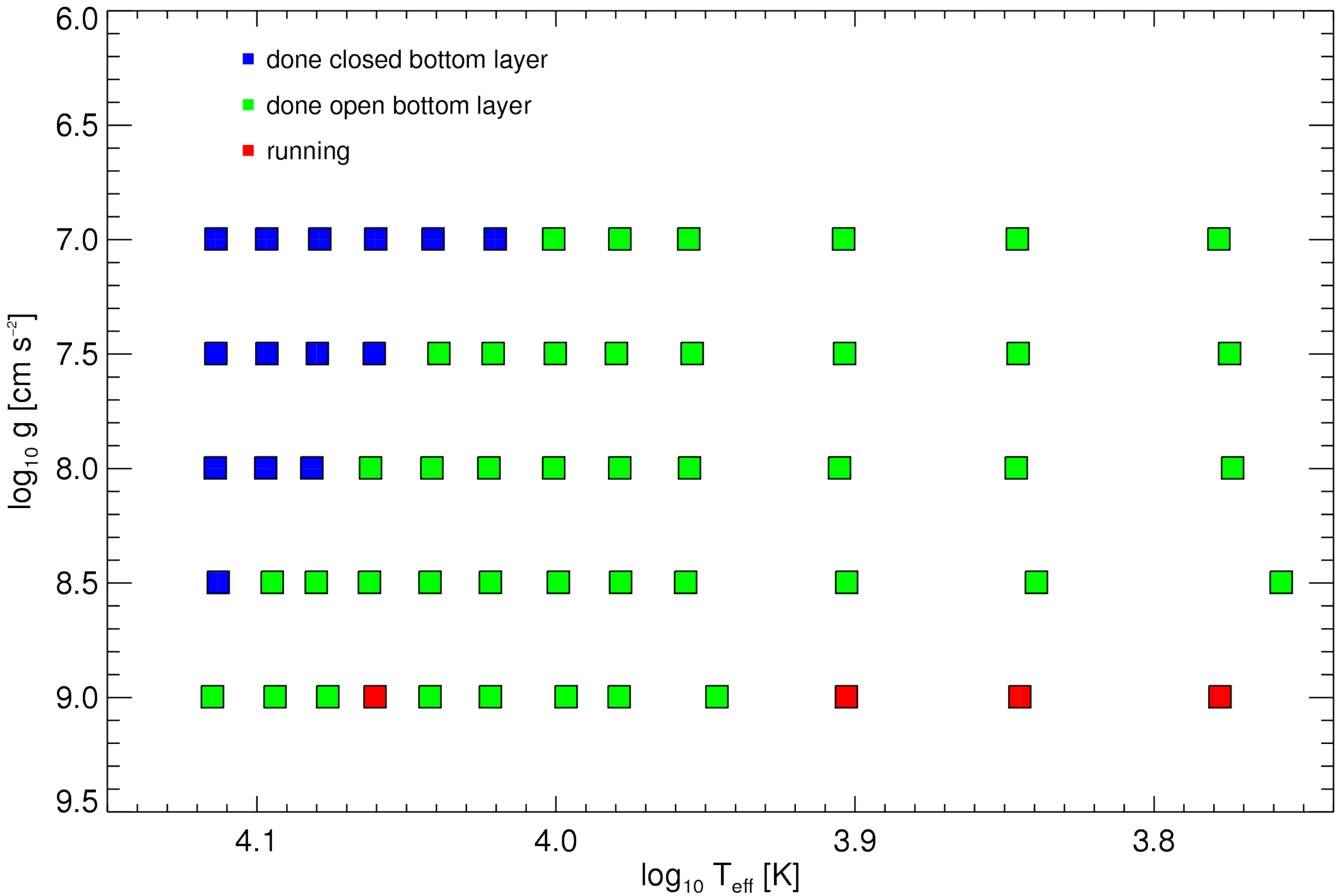
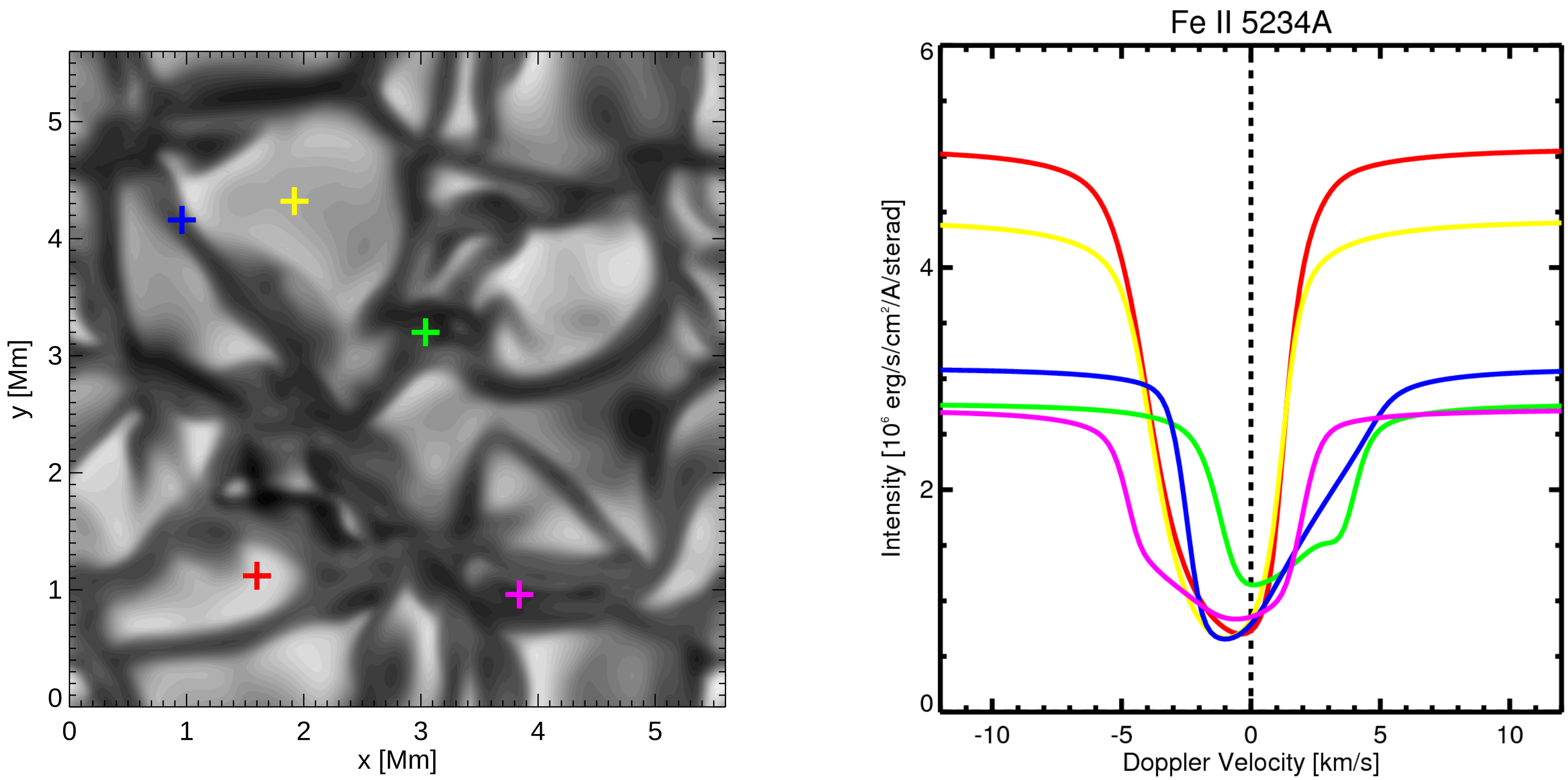


Figure courtesy P.-E. Tremblay

- Ongoing: grid of helium rich (DB) white dwarfs

3D spectral line formation with the `Linfor3D` package



- Variations in line strength, width, shift, asymmetry across granulation pattern
- Non-linearities cause net effects in disk-integrated light
- Knowledge of detailed line shapes → no micro/macro-turbulence
- Ongoing: adding departures from LTE → `NLTE3D` code (Li, O, soon more)

CO^{5}BOLD **3D abundances (E. Caffau) in comparison to others**

EL	N	CO^{5}BOLD	AG89	GS98	AGS05	AGSS09
Li	1	1.02 ± 0.02	1.16 ± 0.10	1.10 ± 0.10	1.05 ± 0.10	1.05 ± 0.10
C	43	8.50 ± 0.11	8.56 ± 0.04	8.52 ± 0.06	8.39 ± 0.05	8.43 ± 0.05
N	12	7.86 ± 0.12	8.05 ± 0.04	7.92 ± 0.06	7.78 ± 0.06	7.83 ± 0.05
O	10	8.76 ± 0.07	8.93 ± 0.035	8.83 ± 0.06	8.66 ± 0.05	8.69 ± 0.05
P	5	5.46 ± 0.04	5.45 ± 0.04	5.45 ± 0.04	5.36 ± 0.04	5.41 ± 0.03
S	9	7.15 ± 0.06	7.21 ± 0.06	7.33 ± 0.11	7.14 ± 0.05	7.12 ± 0.03
Eu	5	0.52 ± 0.03	0.51 ± 0.08	0.51 ± 0.08	0.52 ± 0.06	0.52 ± 0.04
Hf	4	0.87 ± 0.04	0.88 ± 0.08	0.88 ± 0.08	0.88 ± 0.08	0.85 ± 0.04
Th	1	0.08 ± 0.03	0.12 ± 0.06	*0.09 ± 0.02*	*0.06 ± 0.05*	0.02 ± 0.10
K	6	5.10 ± 0.09	5.12 ± 0.13	5.12 ± 0.13	5.08 ± 0.07	5.03 ± 0.09
Fe	15	7.51 ± 0.08	7.67 ± 0.03	7.50 ± 0.05	7.45 ± 0.05	7.50 ± 0.04
Os	3	1.15 ± 0.06	1.45 ± 0.10	1.45 ± 0.10	1.45 ± 0.10	1.25 ± 0.07
Z		$\boxed{0.0154}$	$\boxed{0.0189}$	0.0171	$\boxed{0.0122}$	0.0134
Z/X		0.0211	0.0267	0.0234	0.0165	0.0183

AG89 Anders & Grevesse Geochemica et Cosmochimica acta, 1989 Vol. 53 (6th place)

GS98: Grevesse et Sauval; Space Science Reviews 85: 161-174, 1998

AGS05: Asplund et al.; ASP Conferences Series, Vol. 336, 2205

AGGS09: Asplund, Grevesse, Sauval, & Scott, 2009, ARAA 47, 481

At tension: photospheric abundances and helioseismic inferences

- Over the last decade refined analysis of solar photospheric abundances by Asplund+ and Caffau+ led to downward revision of CNO elements by $\approx 1/3$
  - reflects on metal content of present day Universe
- p-mode frequencies predicted by standard solar models significantly off with low metal abundances while ok with older, higher metal abundances
- Opacity at bottom of surface convection zone (CZ) crucial
- Increase of mean (Rosseland) opacity by $\approx 15\,\%$ could resolve the issue
  - OPAL and OP people were convinced that the opacity cannot be off by this amount
  - main opacity contributor oxygen $\rightarrow$ simple, hydrogenic ion at base of CZ
  - iron provides $\approx 1/4$ of mean opacity
- Many extensions (B-fields, non-standard mixing, ...) of standard models were discussed without convincing resolution of the problem

LETTER

doi:10.1038/nature14048

A higher-than-predicted measurement of iron opacity at solar interior temperatures

J. E. Bailey[1], T. Nagayama[1], G. P. Loisel[1], G. A. Rochau[1], C. Blancard[2], J. Colgan[3], Ph. Cosse[2], G. Faussurier[2], C. J. Fontes[3], F. Gilleron[2], I. Golovkin[4], S. B. Hansen[1], C. A. Iglesias[5], D. P. Kilcrease[3], J. J. MacFarlane[4], R. C. Mancini[6], S. N. Nahar[7], C. Orban[7], J.-C. Pain[2], A. K. Pradhan[7], M. Sherrill[3] & B. G. Wilson[5]

- Paper (Nature, Jan. 1st, 2015) reports measurements of iron opacity at electron temperatures $T_\mathrm{e} = (1.9 \dots 2.3) \times 10^6\,\mathrm{K}$ and electron densities $n_\mathrm{e} = (0.7 \dots 4.0) \times 10^{22}\,\mathrm{cm}^{-3}$
  - thermodynamic conditions close to the conditions at base of solar CZ
- Dependent on wavelength, iron opacity $30 \dots 400\,\%$ greater than predicted
- Roughly half the needed increase of the mean opacity to resolve discrepancy of p-mode frequencies
  - one could speculate that similar increase for other elements could resolve the issue

LETTER

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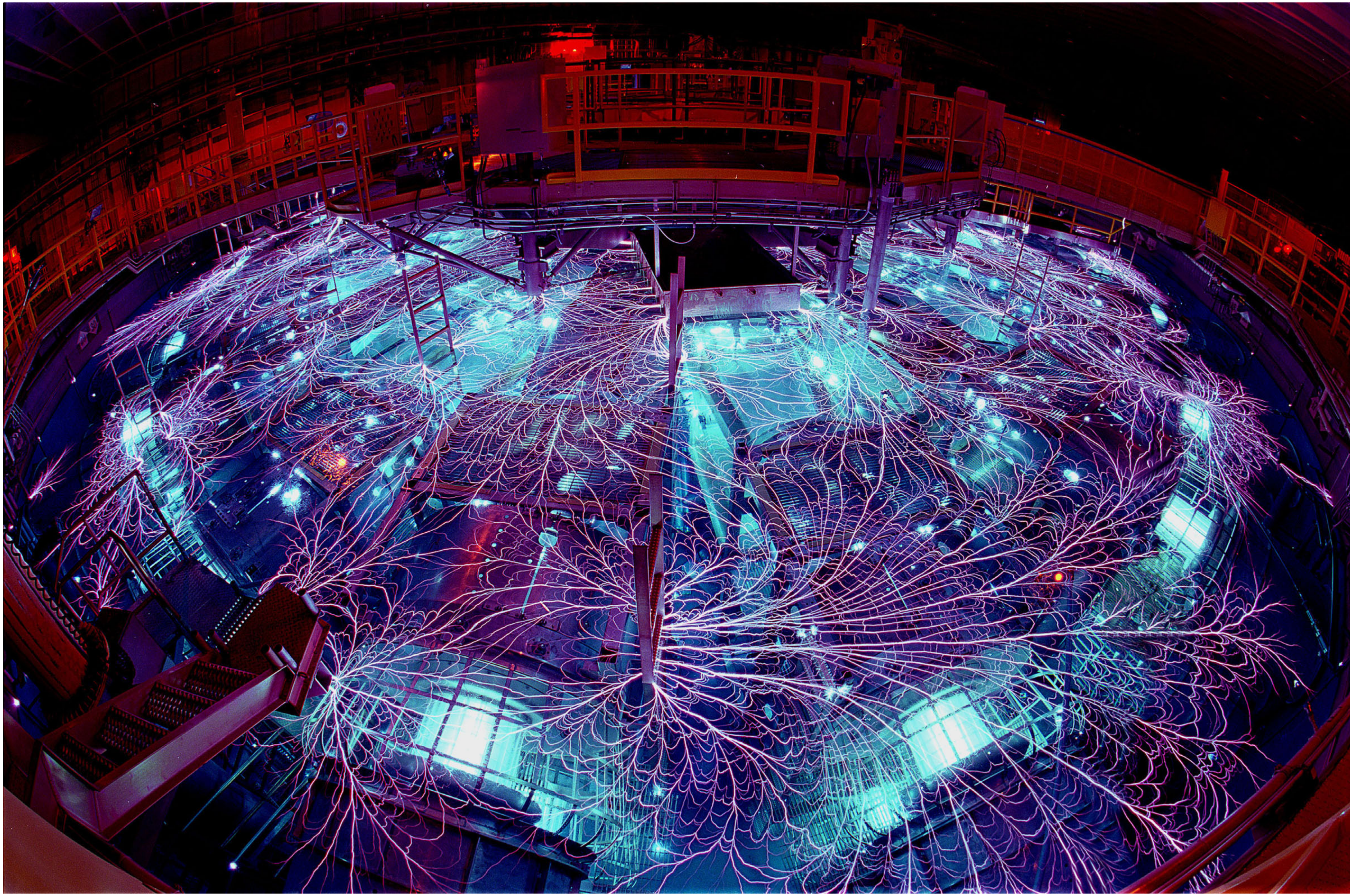
- Central question: how did the experimental physicists pulled this off?
  - can we believe this? what about systematic effects?

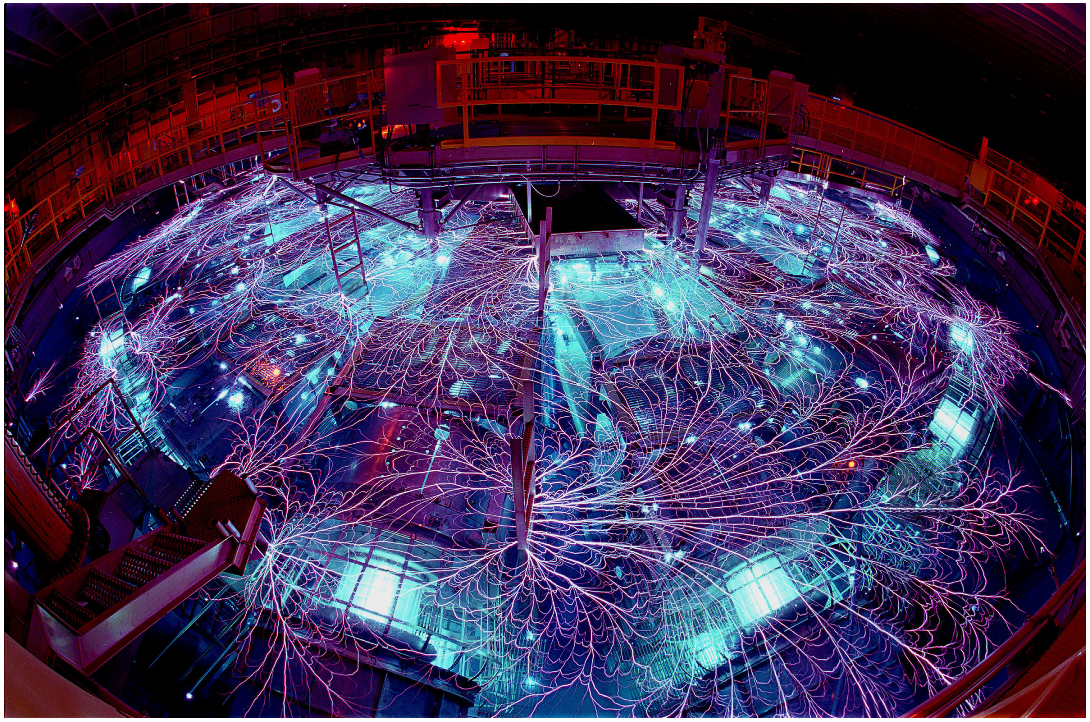
- Two quotes from the paper . . .
  - *The systematic error evaluation comprised the majority of the work conducted for this project.*
  - *The tamper [material embedding the Fe sample] is the only experimental set-up change between the lower-$T_{\mathrm{e}}/n_{\mathrm{e}}$ results that agree reasonably well with opacity calculations.*

The Z-machine . . .

Z Pulsed Power Facility, aka "The Z-machine"



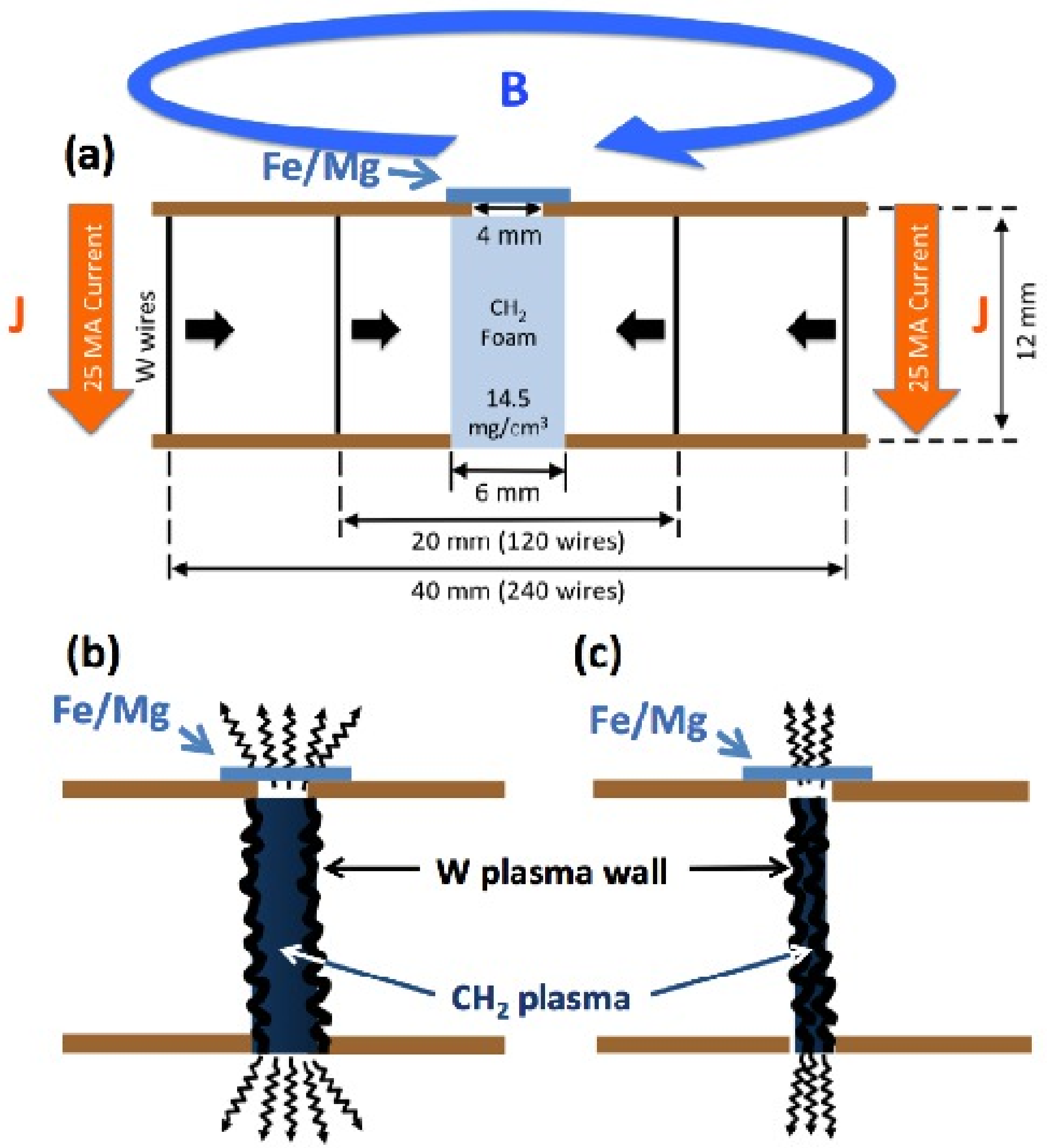
Z Pulsed Power Facility, aka “The Z-machine”



From Wikipedia: Z machine at Sandia National Laboratory. Due to the extremely high voltage, the power feeding equipment is submerged in concentric chambers of 2,000 m^3 of transformer oil and 2,300 m^3 of deionized water, which act as insulators. Nevertheless, the electromagnetic pulse when the machine is discharged causes impressive lightning, referred to as a flashover”, which can be seen around many of the metallic objects in the room.

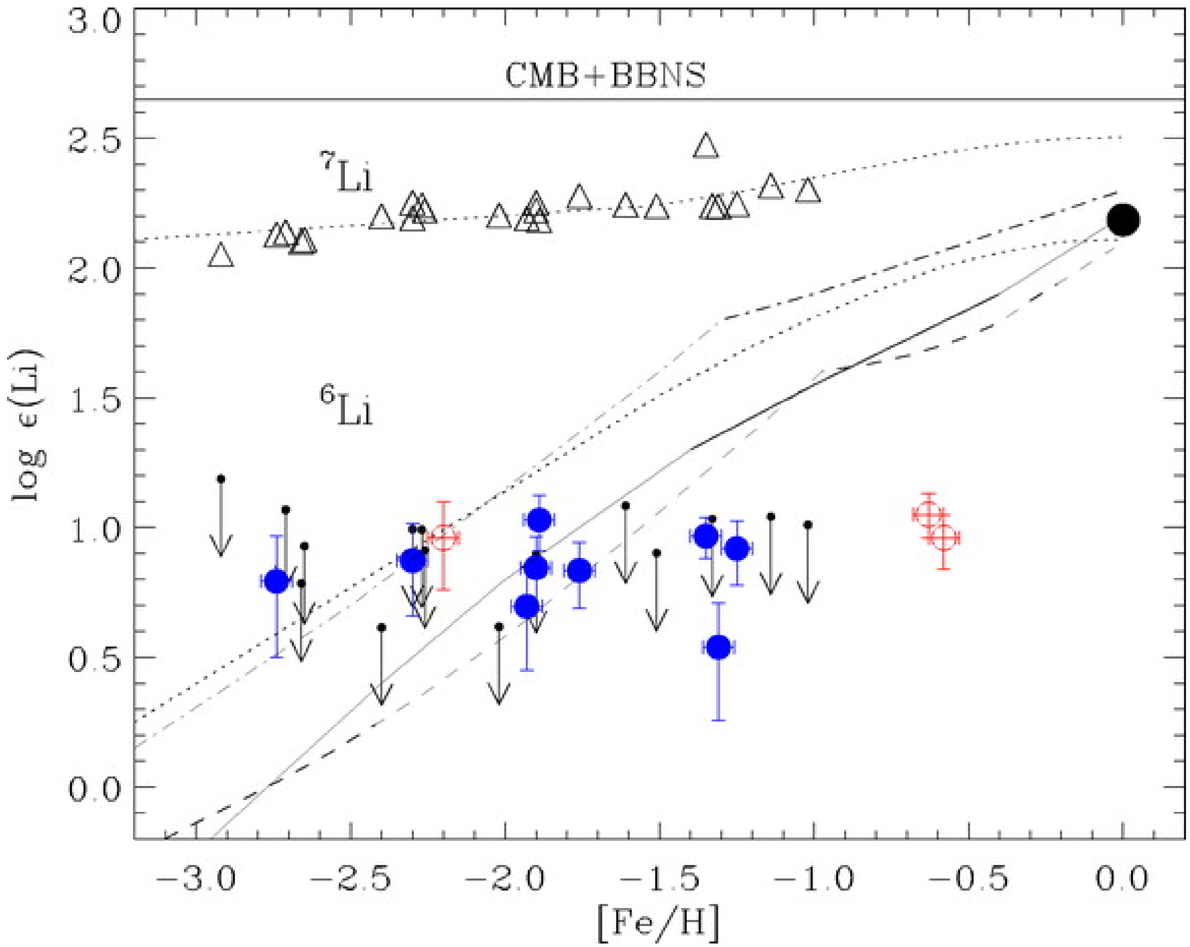
- Z-machine at Sandia National Laboratory largest X-ray generator in the world
- Purpose: testing materials at conditions of extreme temperature and pressure

Z-pinch → shock → heats target → thermal X-ray emitter



(figure from Nagayama et al. 2014)

^{6}Li and ^{7}Li in metal-poor halo stars



(Asplund et al. 2006; Smith et al. 1993, 1998; Cayrel et al. 1999; Nissen et al. 1999; chemical evolution models: Prantzos 2006; Ramaty et al. 2000; Fields & Olive 1999; Vangioni-Flam et al. 2000)

- Not corrected for stellar endogenic depletion; arrows indicate 3σ upper limits
- Apparent detections suggest a plateau of ^{6}Li/^{7}Li isotopic ratio ≈ 0.05

Consequences of ^{6}Li plateau in metal-poor halo stars?

- Standard Big Bang nucleosynthesis makes a clear prediction: there should be essentially no ^{6}Li produced

- At early times spallation of CNO nuclei by cosmic rays should not have contributed much Li

- Situation spawned a lot of subsequent work
  $\rightarrow$ 290 citations of Asplund+ 2006 paper
  - non-standard Big Bang nucleosynthesis
  - touched also on fundamental physics, e.g. number of neutrino flavors

- Largely forgotten: final result of Asplund+ derived from 1D standard models ...

Spectroscopic measurement of ^{6}Li abundance challenging

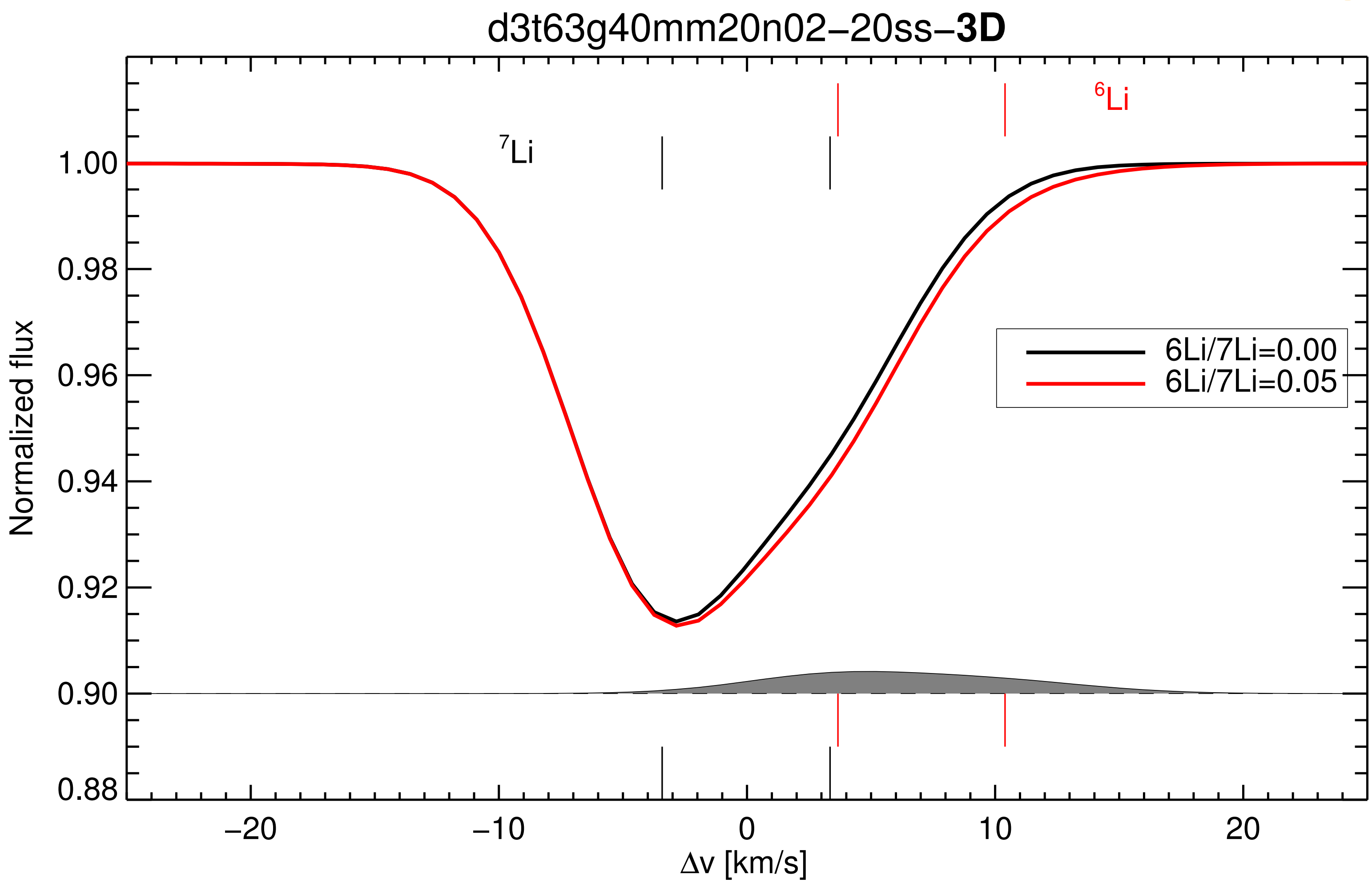
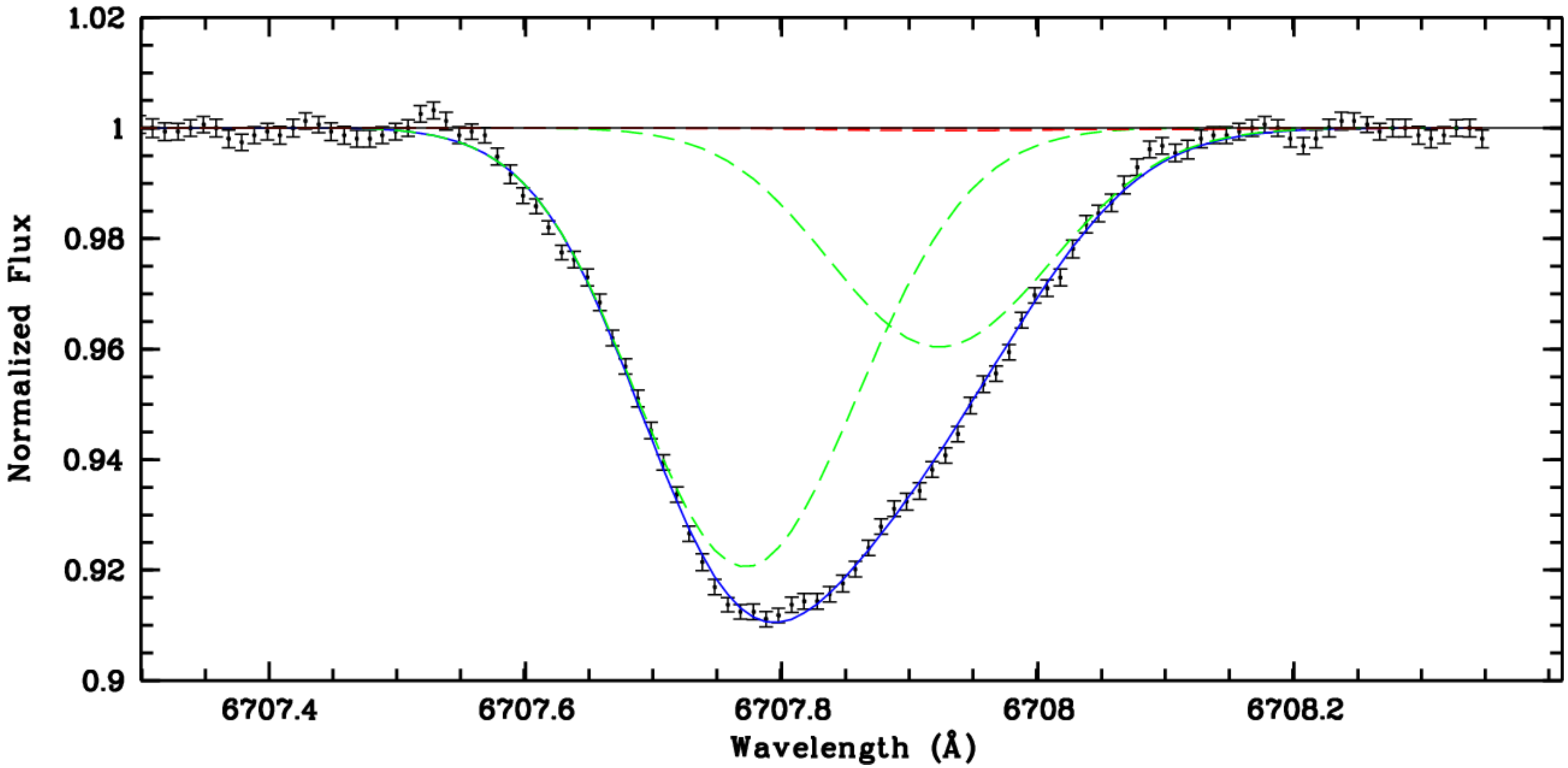


Figure from Steffen et al. 2012

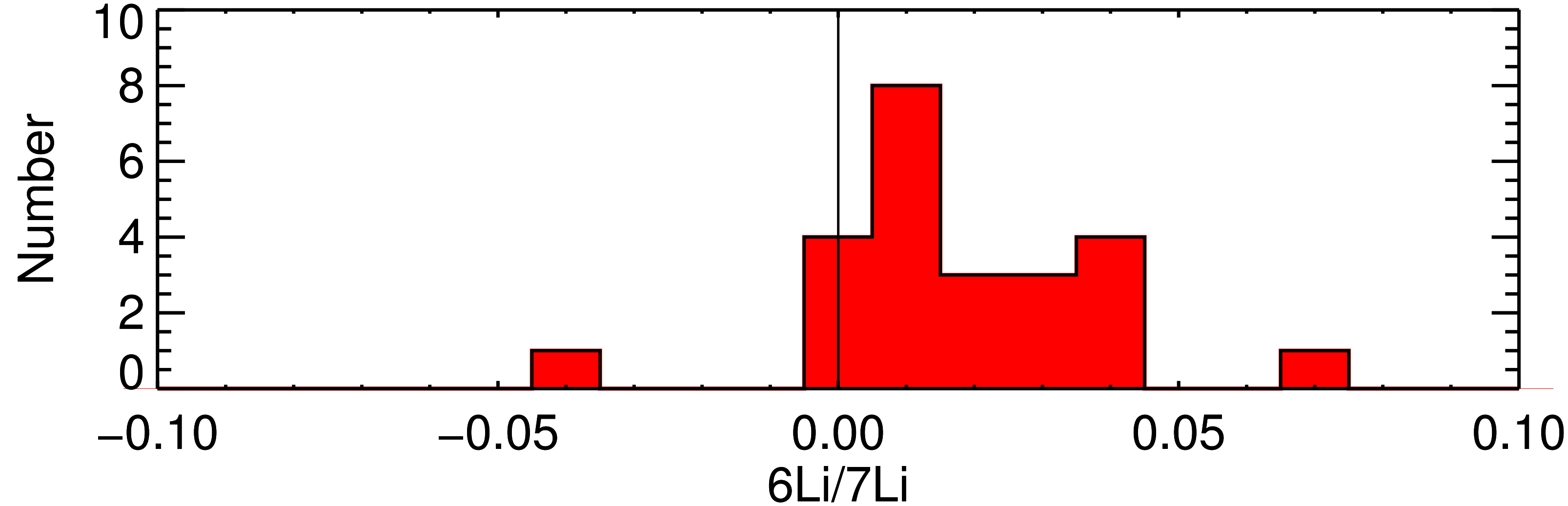
- ^{6}Li produces slight depression in the red wing of a complex blend of ^{7}Li and ^{6}Li
- Convective velocity field produces line asymmetries that can mimic this effect
- Li-feature heavily affected by NLTE effects $\rightarrow$ strength & line shape

Case study (Cayrel et al. 2007): ^{6}Li/^{7}Li isotopic ratio in the metal-poor halo dwarf HD74000



- Outstanding observational material: 20h HARPS, $\lambda/\Delta\lambda \approx 110\,000$, $\mathrm{S/N} \approx 600$
- In contrast to 1D analysis, 3D+NLTE analysis gave a negligible amount of ^{6}Li
- Casts doubts on all previous 1D measurements

Derivation of theoretical corrections of 1D results



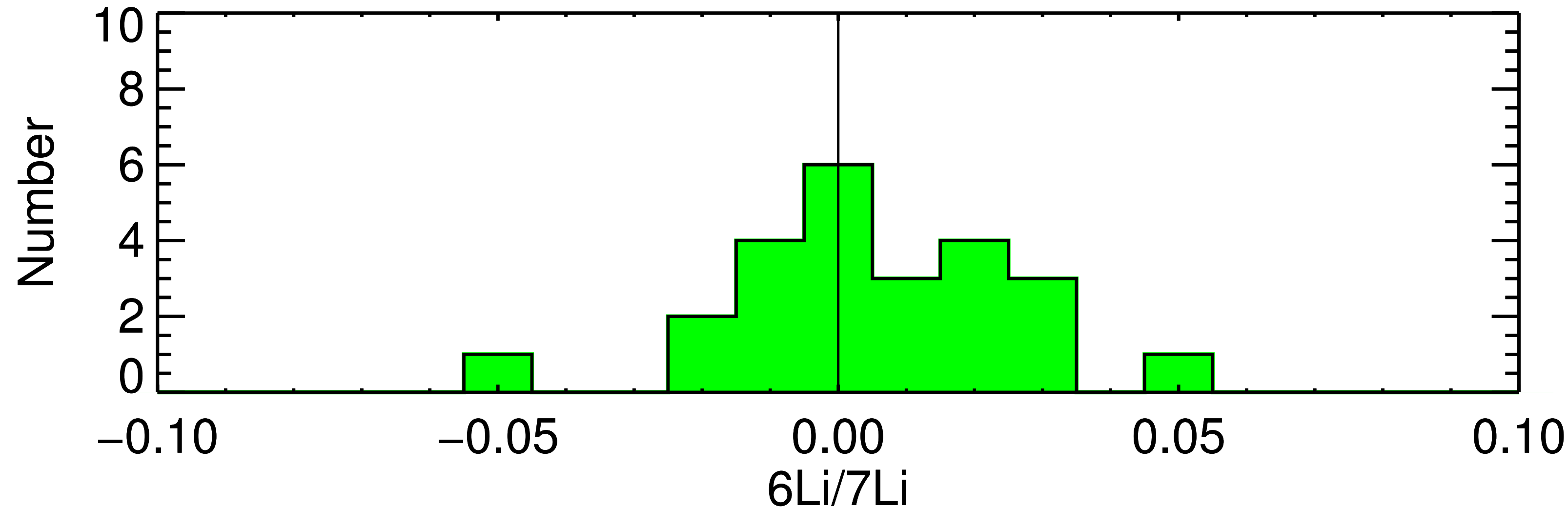


Figure from Steffen et al. 2012

red before correction, green after correction

The lithium isotopic ratio in very metal-poor stars⋆,⋆⋆

K. Lind[1,2], J. Melendez[3], M. Asplund[4], R. Collet[4], and Z. Magic[1]

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ABSTRACT

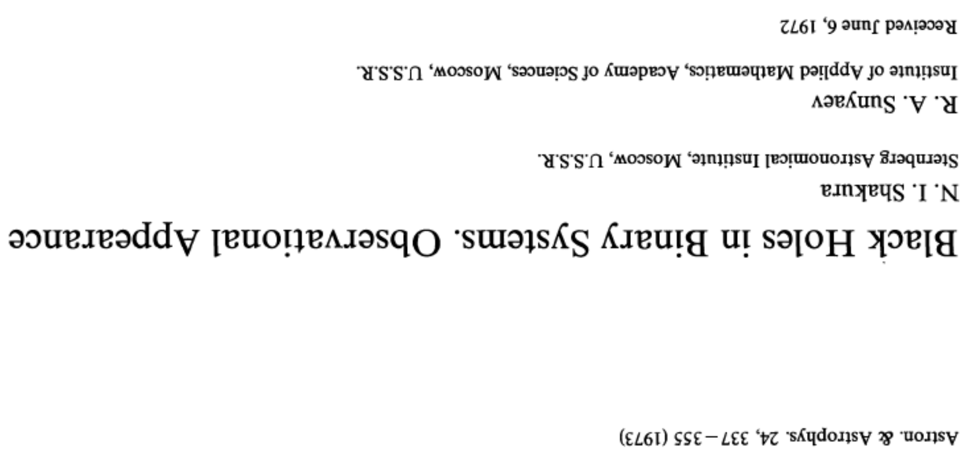
. . .

Conclusions. The observational support for a significant and non-standard ^{6}Li production source in the early universe is substantially weakened by our findings.

- 2013: members of working group of Asplund switched to full 3D+NLTE analysis
- Bottom line: in rare cases ^{6}Li may be present in old, metal-poor halo stars but clearly: ^{6}Li is rather the exception than the rule

Final remarks

- 3D model atmospheres provide a path towards higher accuracy for deriving stellar surface properties
- Sometimes, a new perspective can be provided
- Also application of models in projects where their convective properties and dynamics (time-dependence) are relevant
- And yes, paper no. 5 . . .


Astron. & Astrophys. 24, 337–355 (1973)

Black Holes in Binary Systems. Observational Appearance

N. I. Shakura

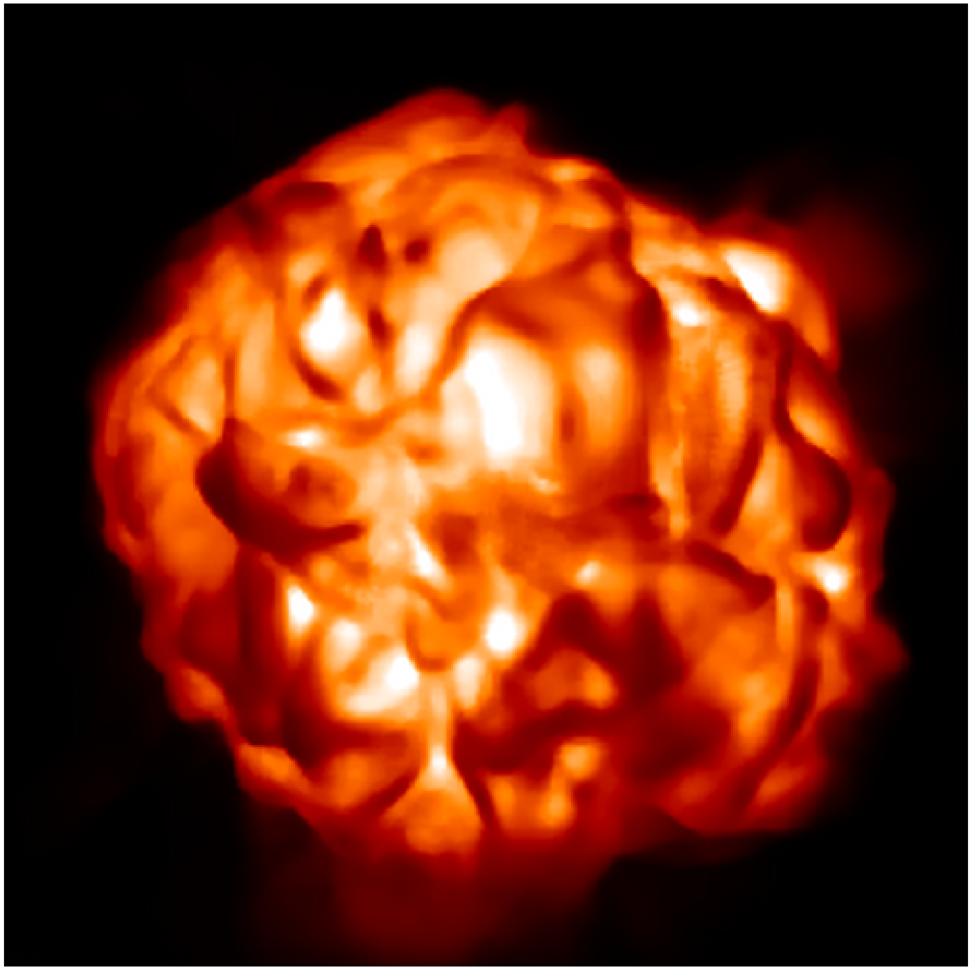
Sternberg Astronomical Institute, Moscow, U.S.S.R.

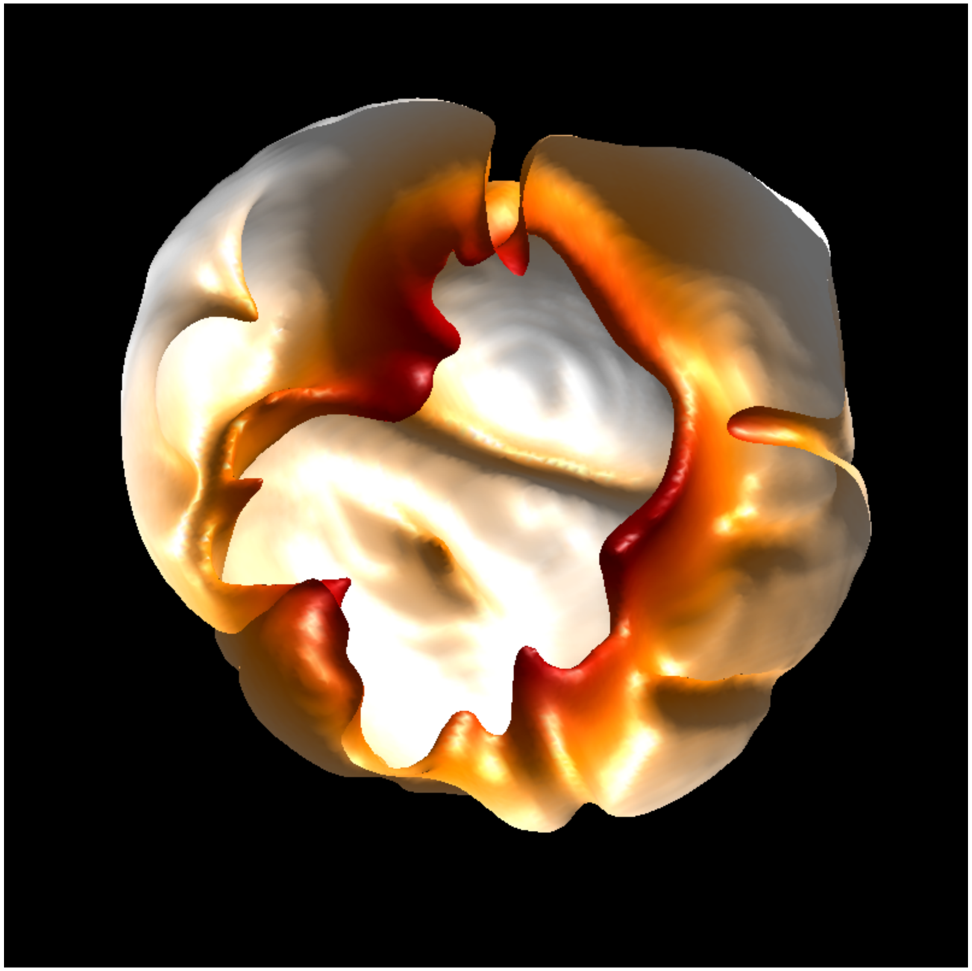
R. A. Sunyaev

Institute of Applied Mathematics, Academy of Sciences, Moscow, U.S.S.R.

Received June 6, 1972

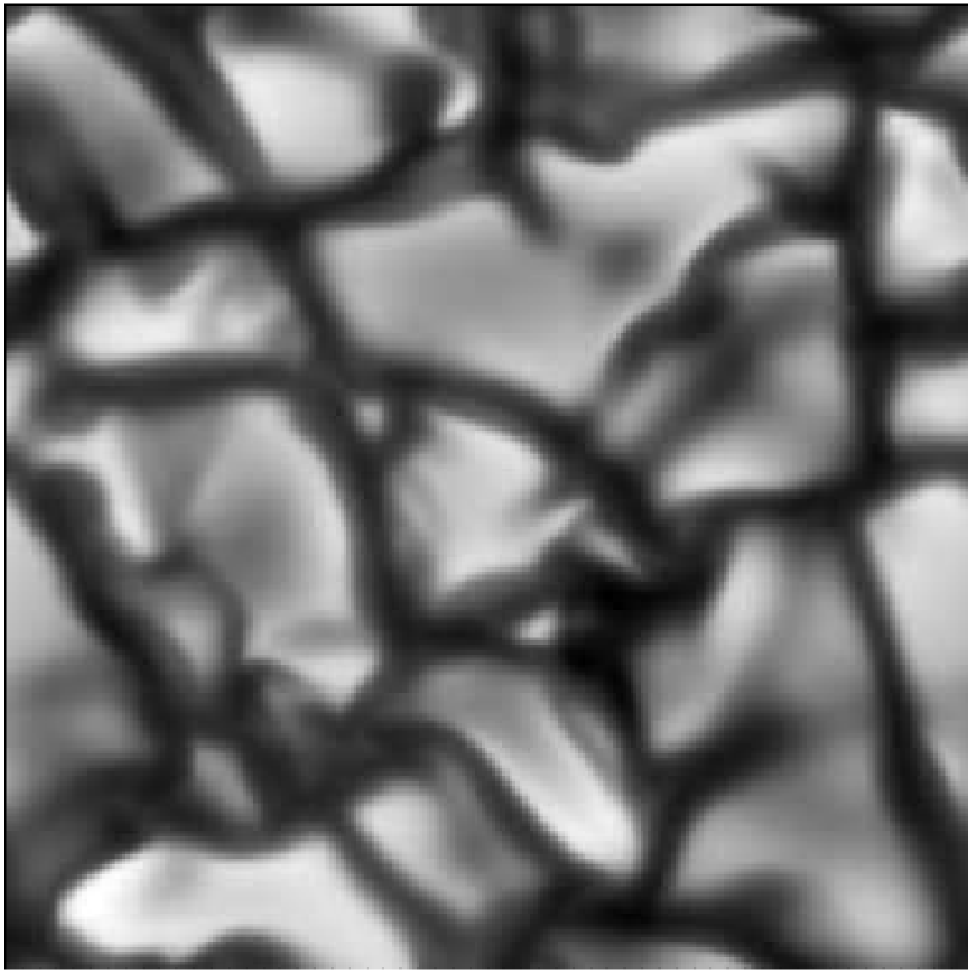
“Star in a Box”



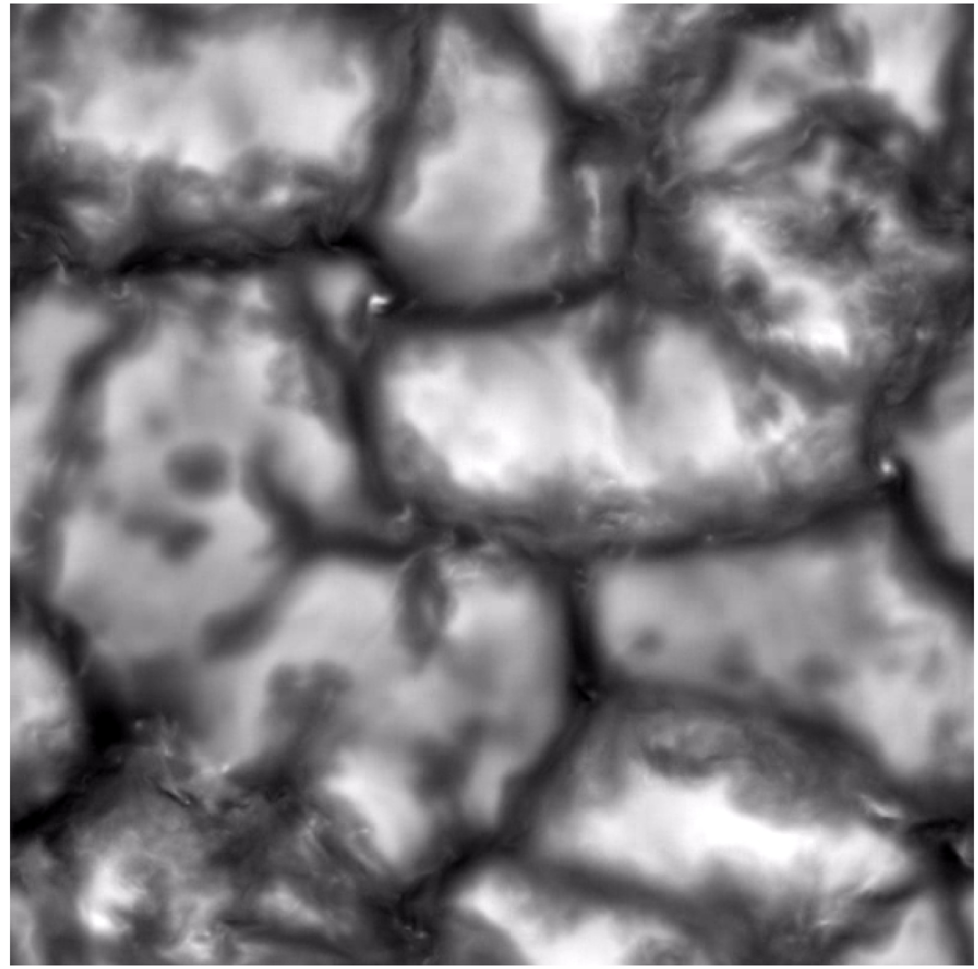


- CO^{5}BOLD model of red supergiant; © B. Freytag (Uppsala)
  - complete stellar envelope, cubic box, Cartesian grid
  - observable radiation intensity (left), entropy-isosurface (right)

Solar granulation at high spatial resolution $\rightarrow$ microturbulence



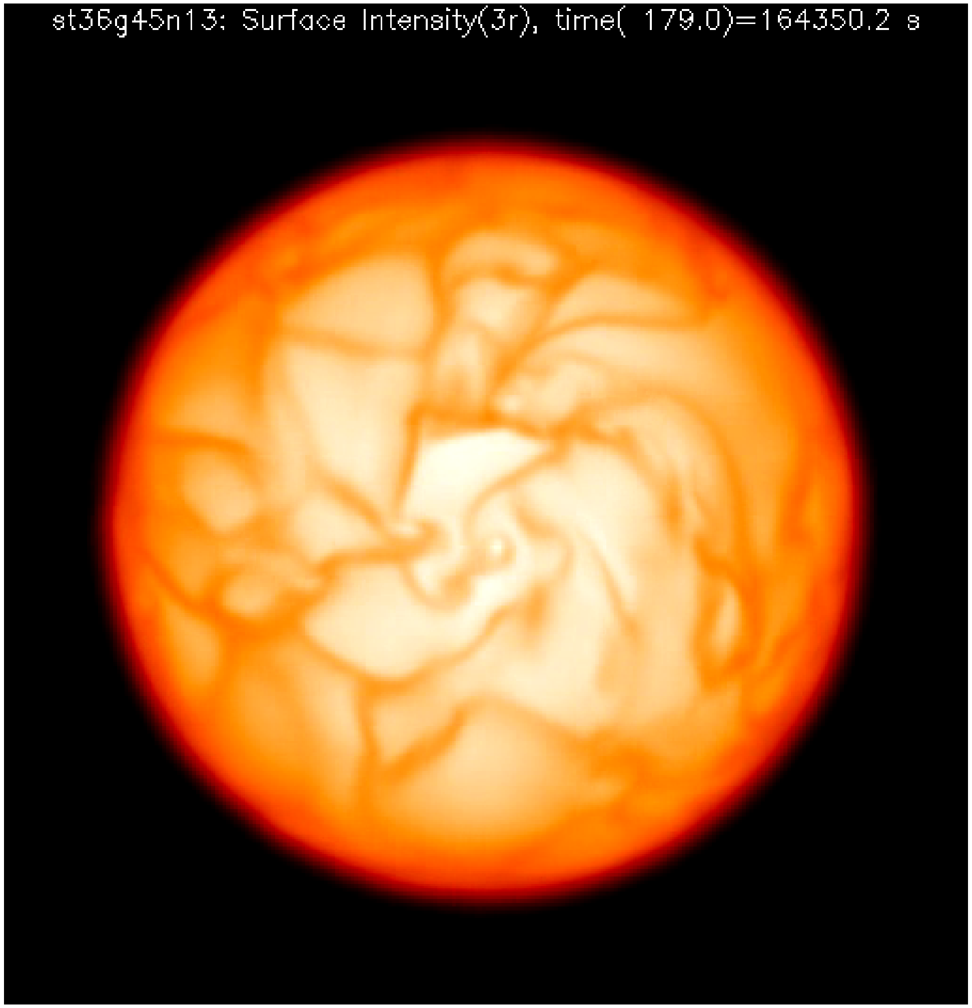
$140 \times 140 \times 150$



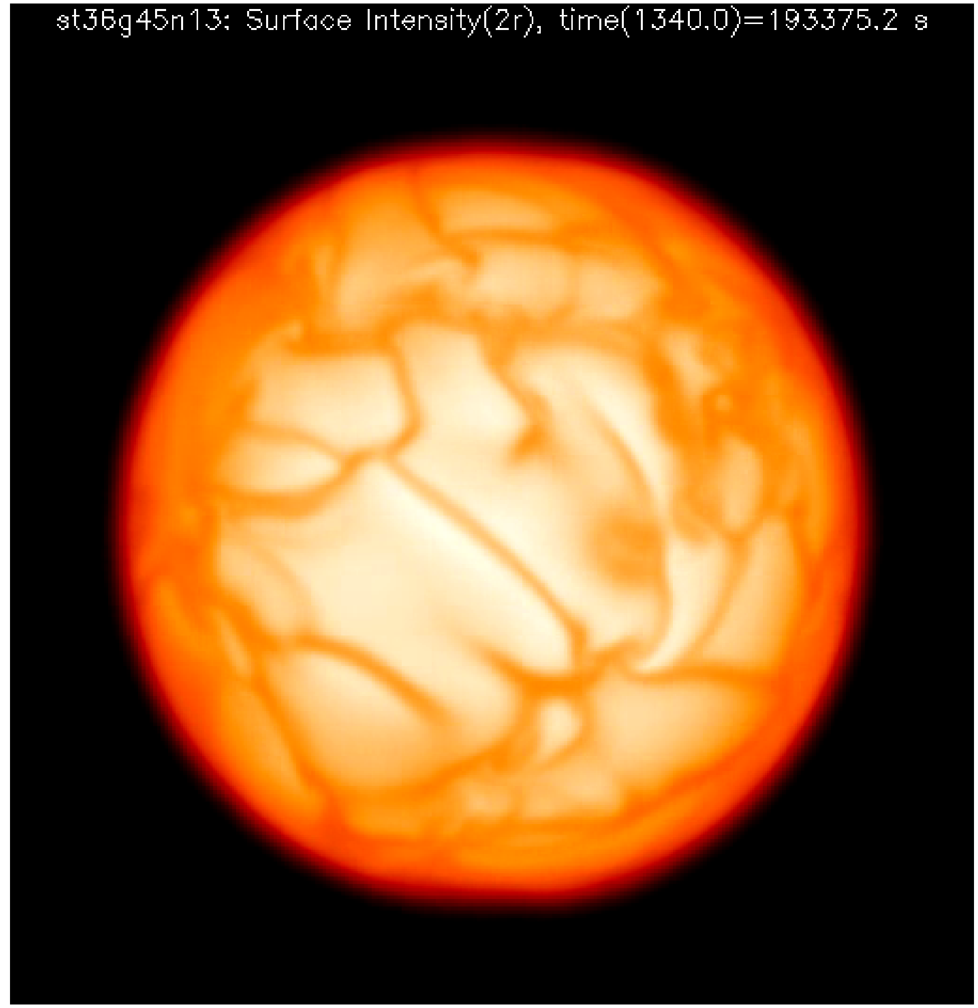
$800 \times 800 \times 400$

- $5.6 \times 5.6 \times 2.8\ \ \mathrm{Mm}^3$, $7\,\mathrm{km}$ cubes, grey radiative transfer
- piecewise parabolic reconstruction $\rightarrow$ low numerical viscosity

Toy model convection-rotation interaction $\rightarrow \alpha_{\mathrm{MLT}}$



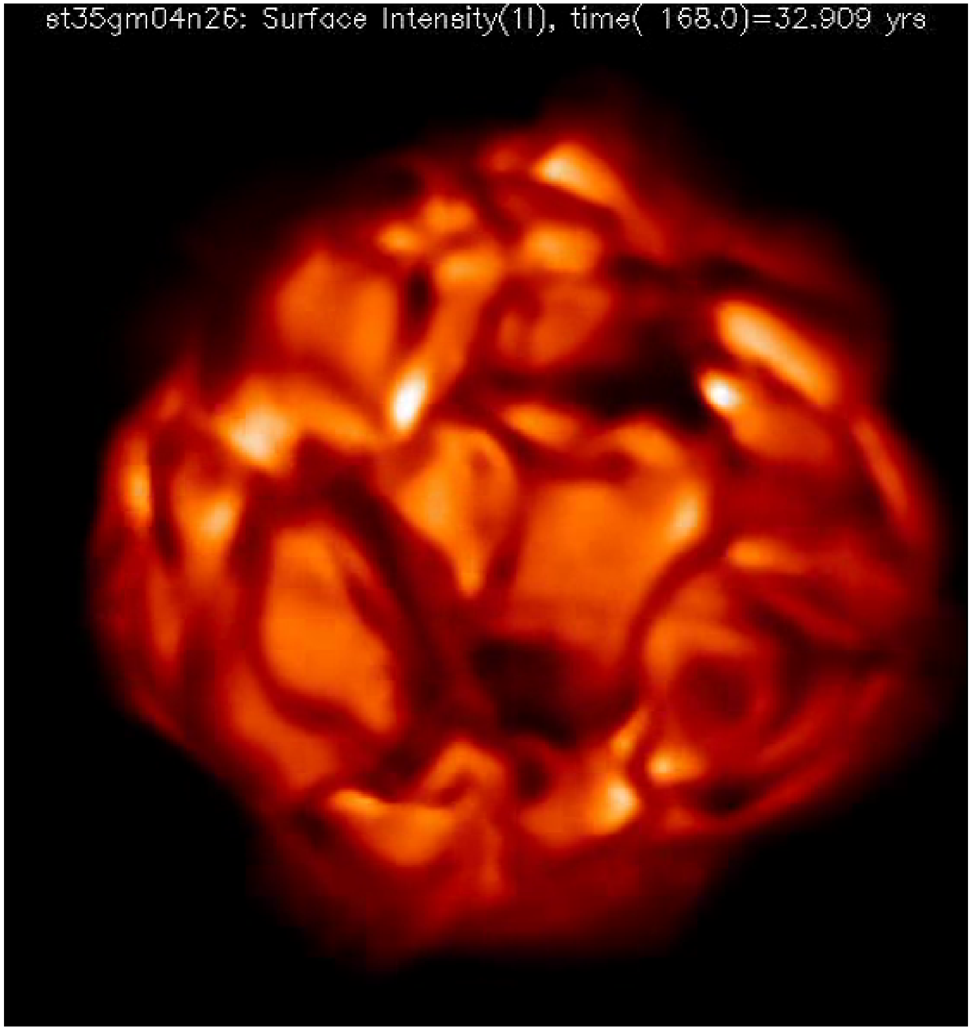
pole-on



equator-on

- T_{eff}=3600 K, $\log g$=4.5, prescribed gravitational potential, 2000 km radius, 255^3 voxels, density contrast $\approx 10^3$, grey radiative transfer
- Coriolis forces only, co-rotating reference frame, $T_{\mathrm{rot}} = 2000\,\mathrm{s}$, $\frac{1}{4}$ break-up

Magnetic field amplification in a red supergiant envelope



- $R \approx 630\, R_\odot$, $L \approx$ several $10^4 L_\odot$, 315^3 voxels
- start with square magnetic loop in center, opacity proportional B

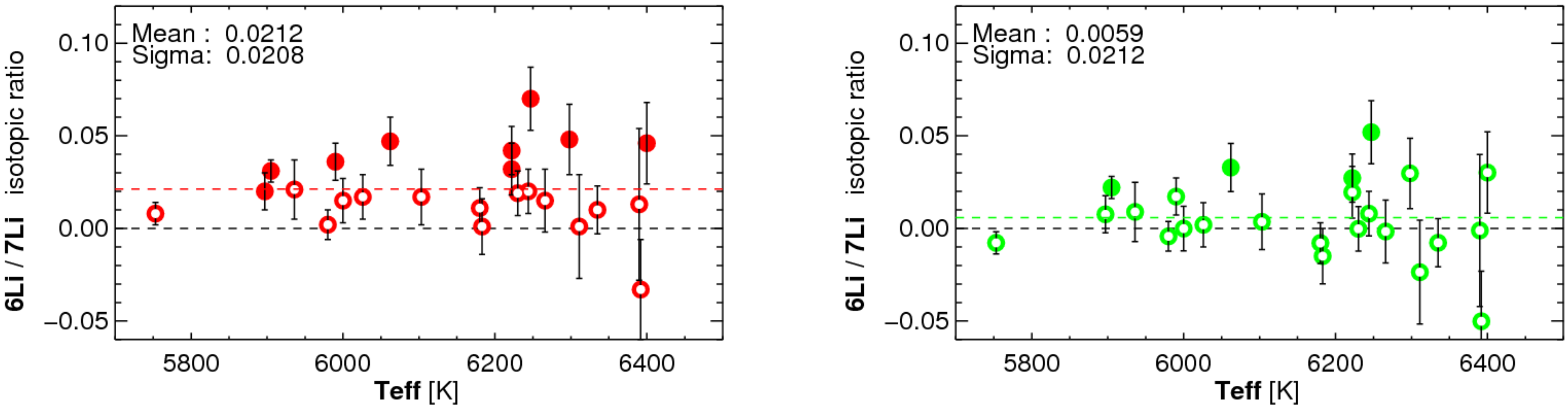
Balance between convective (adiabatic) and radiative equilibrium

$$t_{\mathrm{rad}} = \frac{c_{\mathrm{p}}}{16\sigma\, T^3\, \chi}$$

$$t_{\mathrm{con}} = \frac{H_{\mathrm{p}}}{v_{\mathrm{con}}}$$

- Lack of metal lines in metal-poor atmospheres: $\chi\downarrow \quad t_{\mathrm{rad}}\uparrow$
- T and $\chi(\rho,T)$ dependence causes rapid transition to cool state
- Larger H_{p} at lower gravities makes giants less prone to deviations from radiative equilibrium
  - v_{con} not largely different between dwarfs and giants
  - t_{rad} not sensitively dependent on density

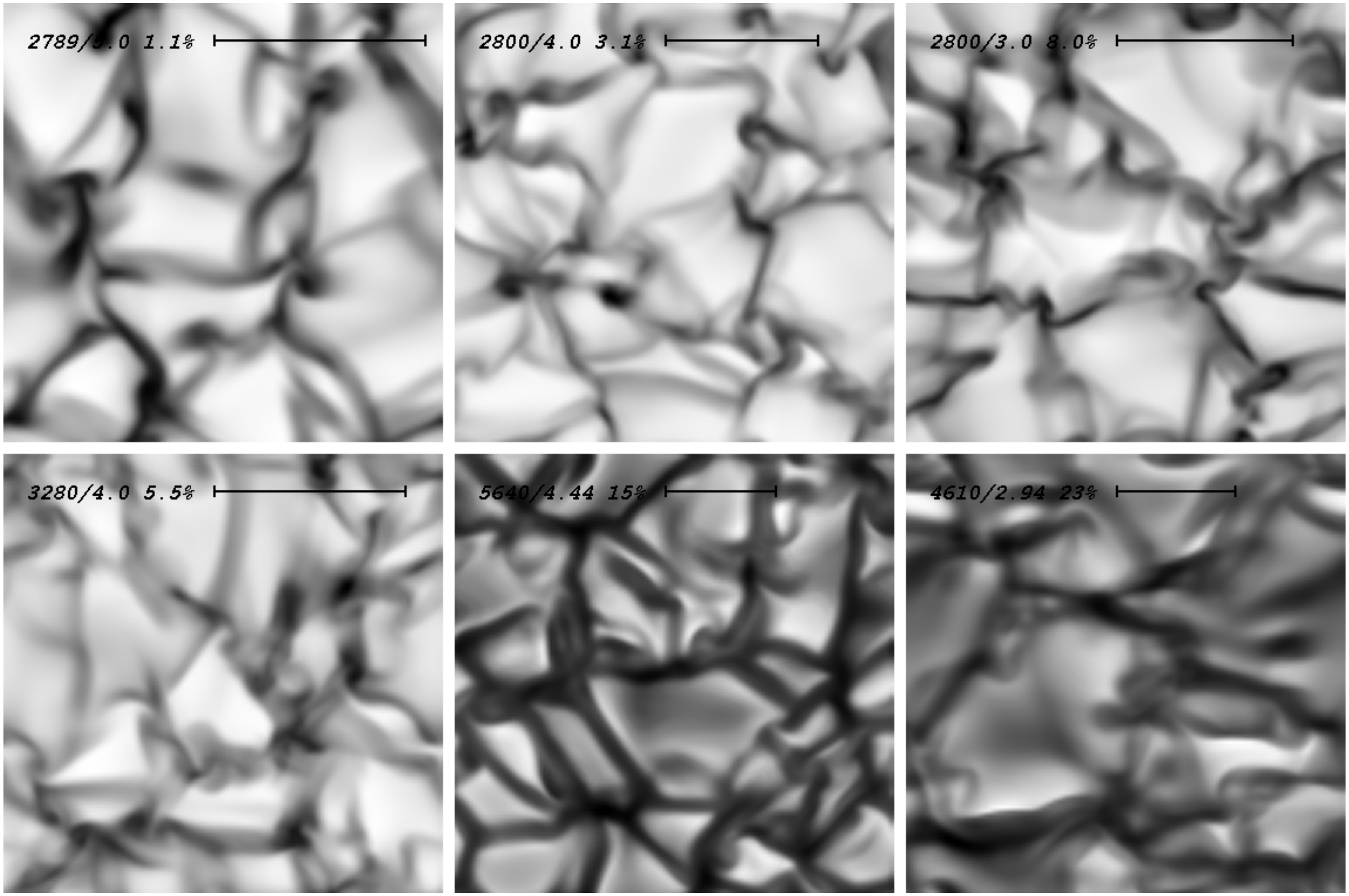
Detections when accounting for 3D and NLTE effects



solid: detections / open: non-detections / left: Asplund et al. 2006 / right: corrected

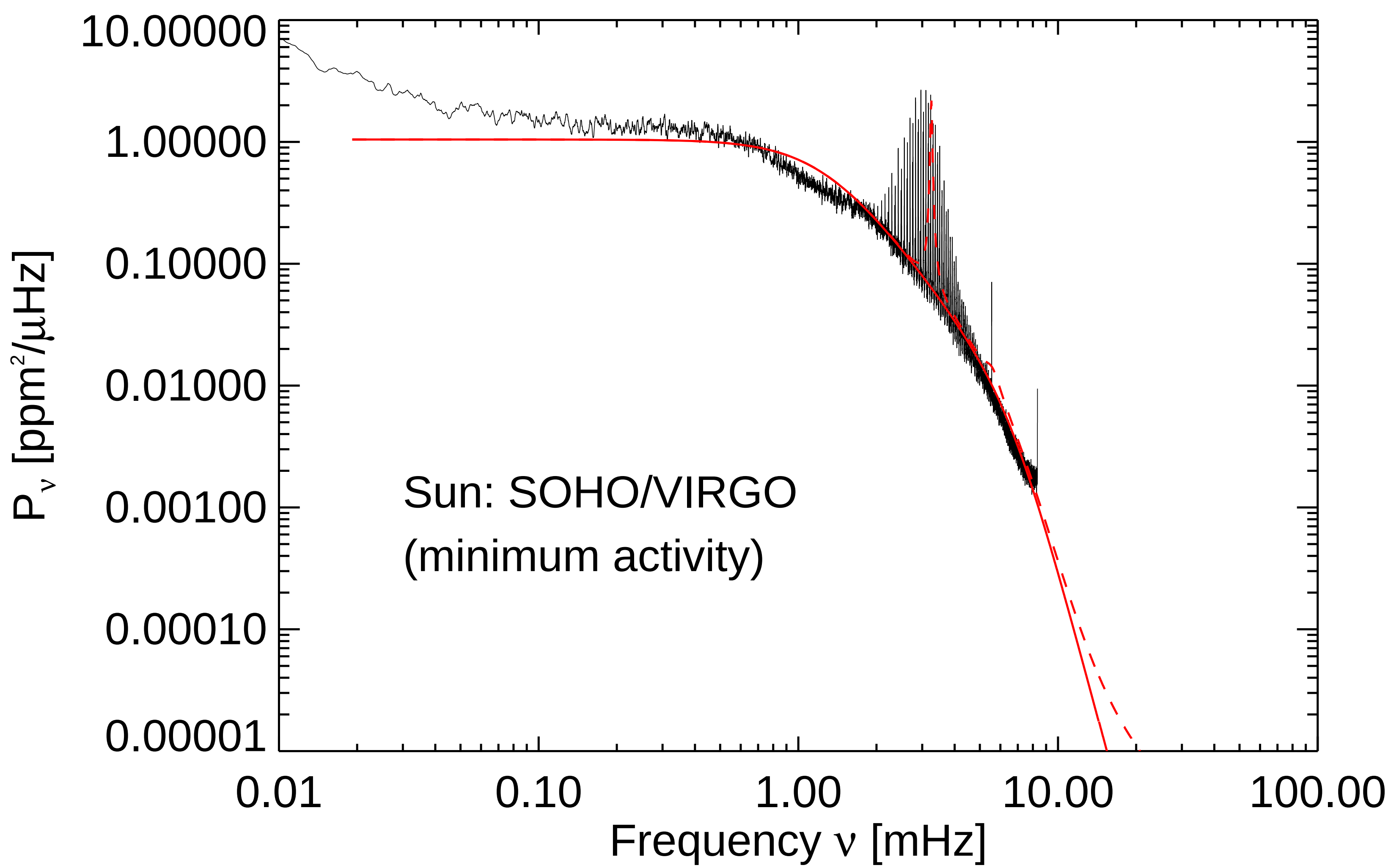
- Reduction from 9 to 2-4 detections out of 24 2σ observations
- ^{6}Li in metal-poor halo stars rather the exception than the rule

3D models of M-type atmospheres



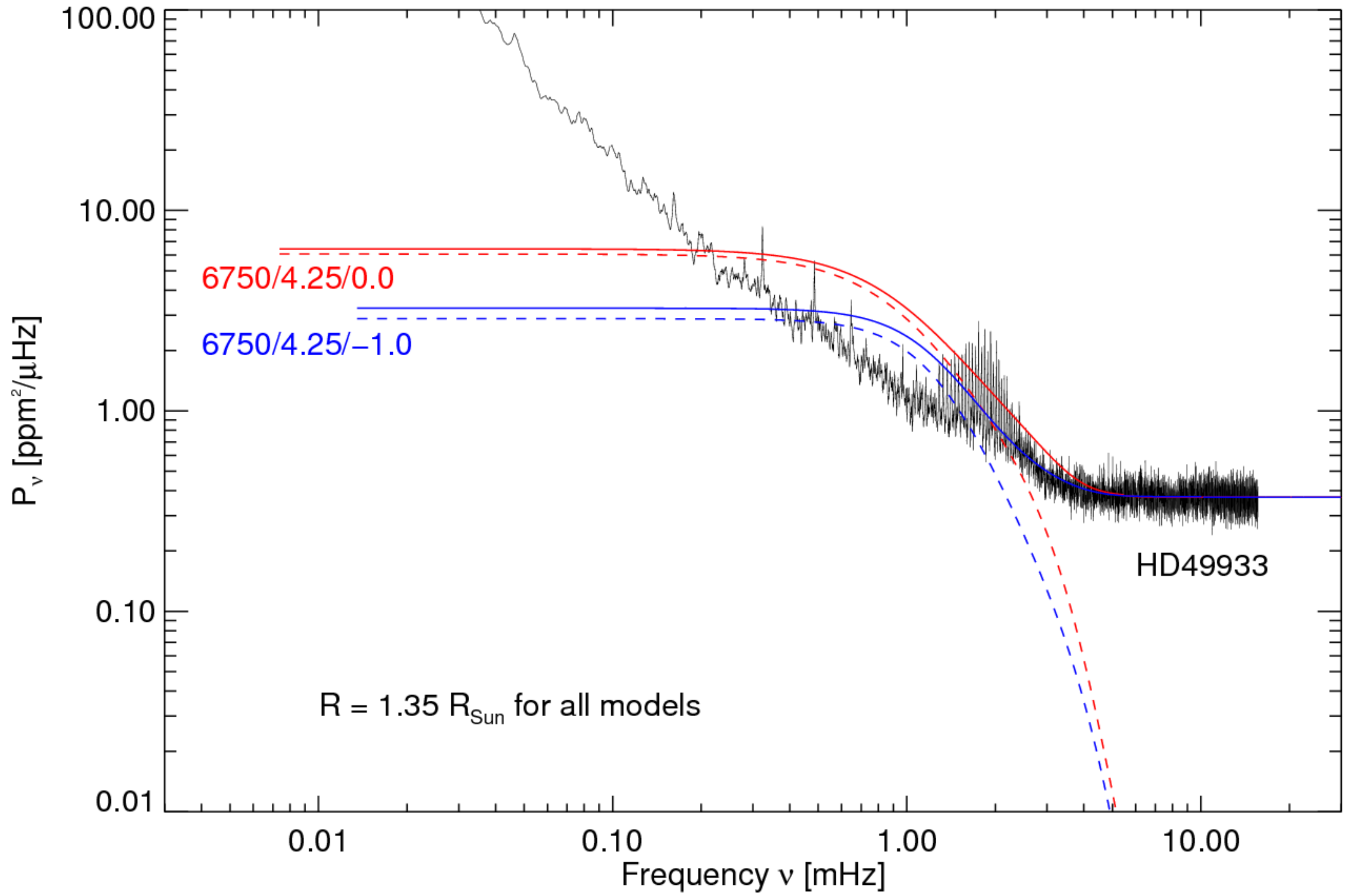
- Follow-up study on turbulence properties and FeH molecular formation
- Opacities for MHD modelling efforts of M-dwarf chromospheres
  $\rightarrow$ talk of S. Wedemeyer

3D models & micro-variability: Sun seen by SOHO/VIRGO



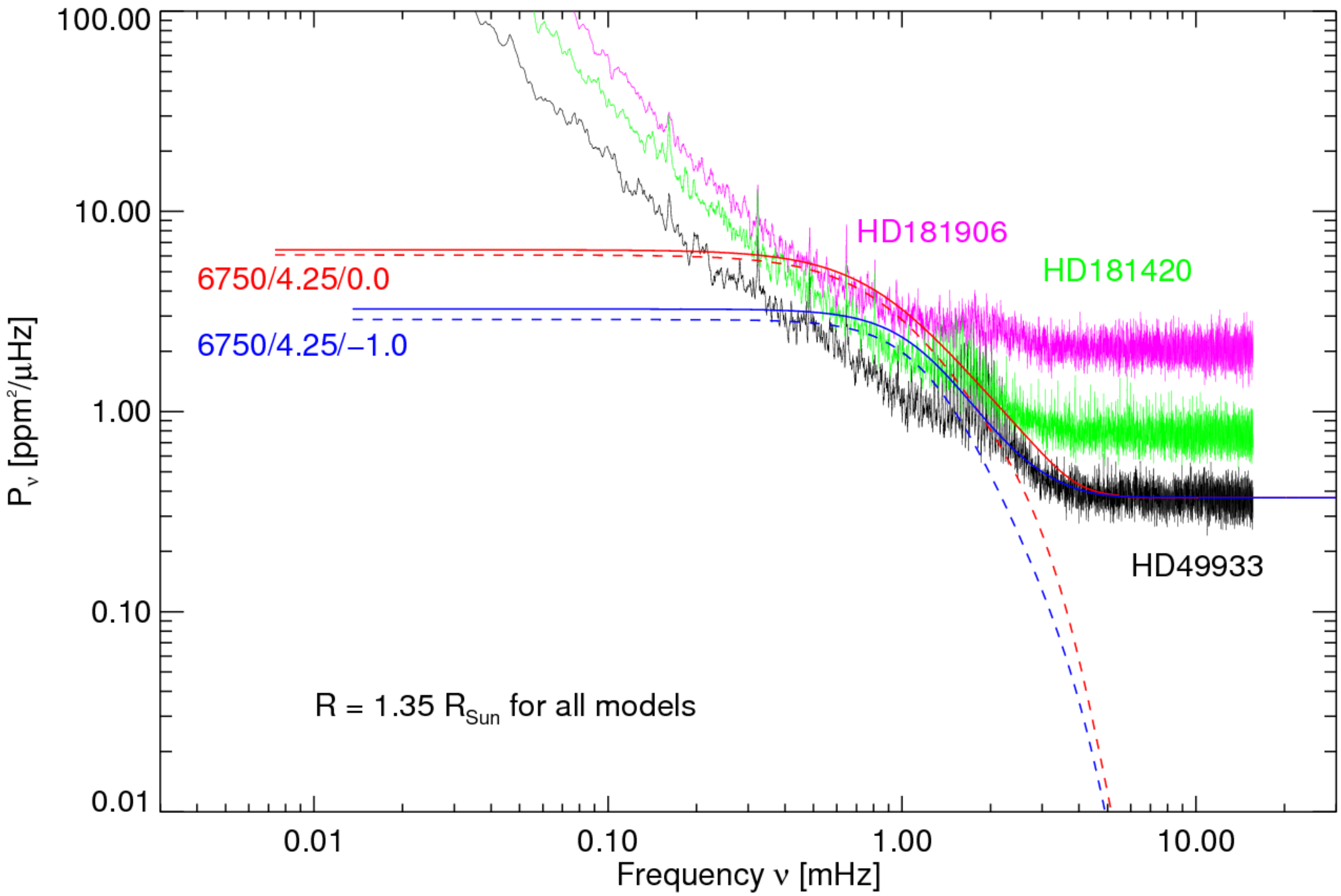
- 3D prediction of granultaion background: satisfactory run of continuum, eigenmodes not directly comparable, absolute scale!
- Magnetic activity dominates signal towards low frequencies

Predictions for COROT's main target HD49933 ([Fe/H]≃-0.40)



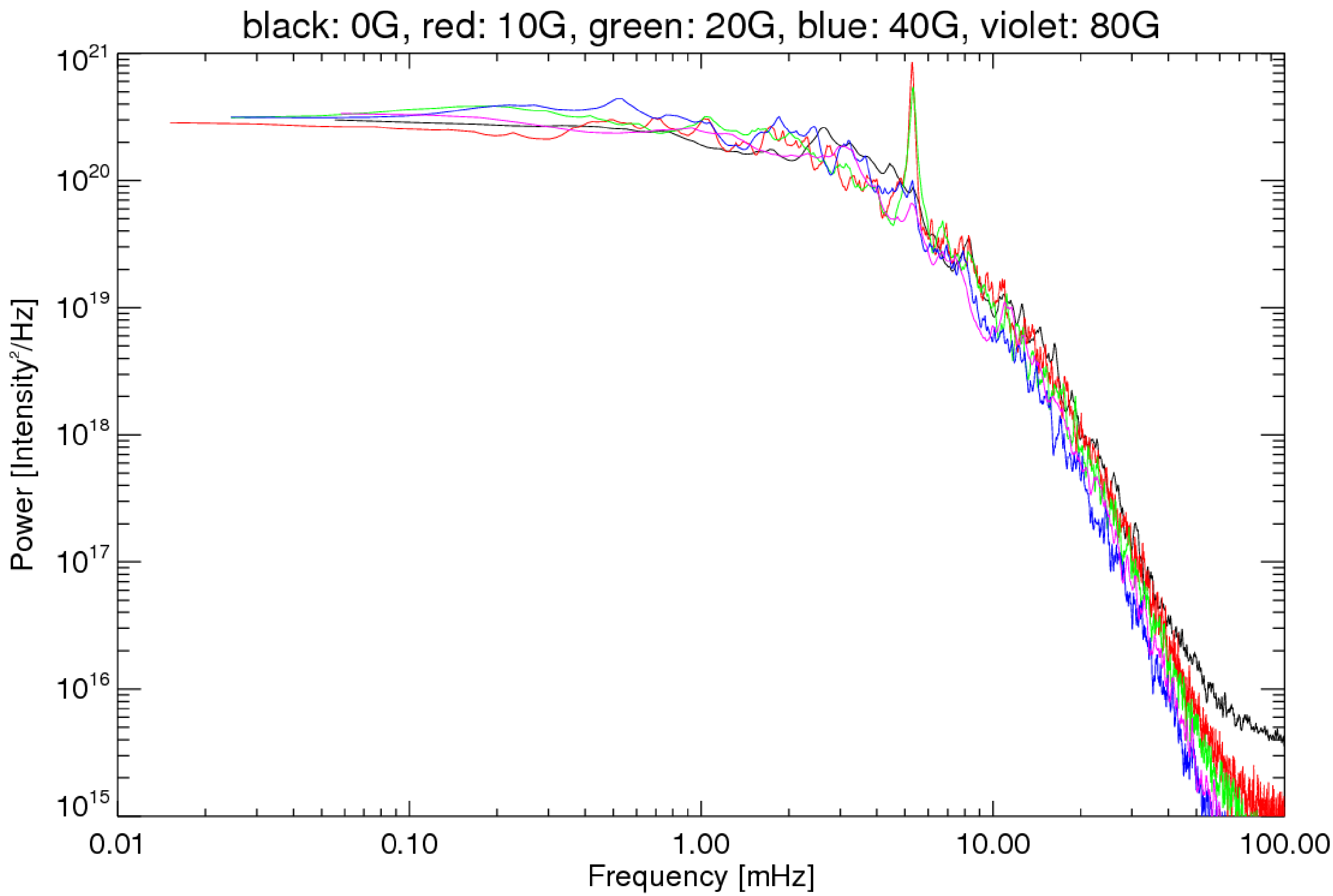
- Bolometric background signal stronger in p-mode region than observed
- Shape of the power spectrum not well matched: activity? local dynamo?

HD49933 does not seem to be an exceptional case



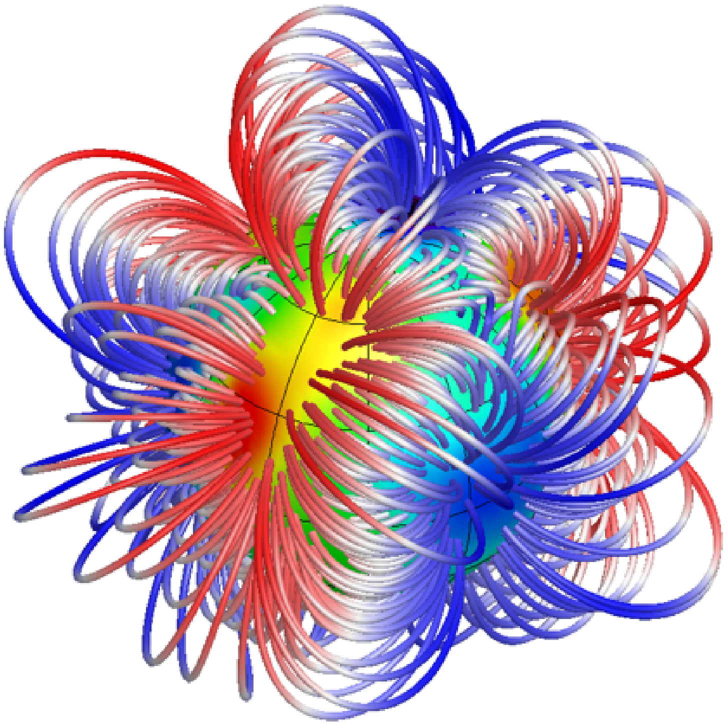
HD49933	$T_{\mathrm{eff}}/\mathrm{K} =$ 6750	$\log g =$ 4.24	[Fe/H] = -0.40
HD181420	6650	4.17	-0.04
HD181906	6380	4.15	-0.14

Lightcurves of solar 2D MHD runs of increasing magnetic flux



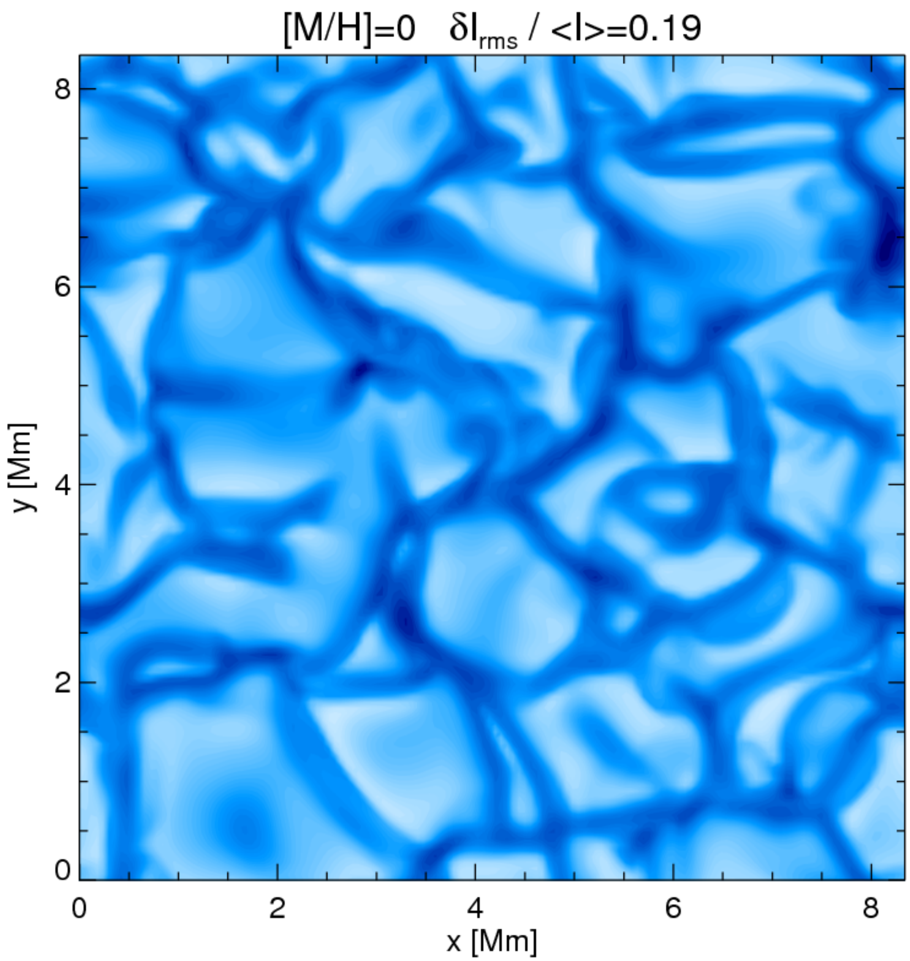
- Change of granular dynamics by magnetic field mainly influences highest frequencies
- Polarization: no globally organized magnetic field on 1 G level (C. Catala, p.comm.)

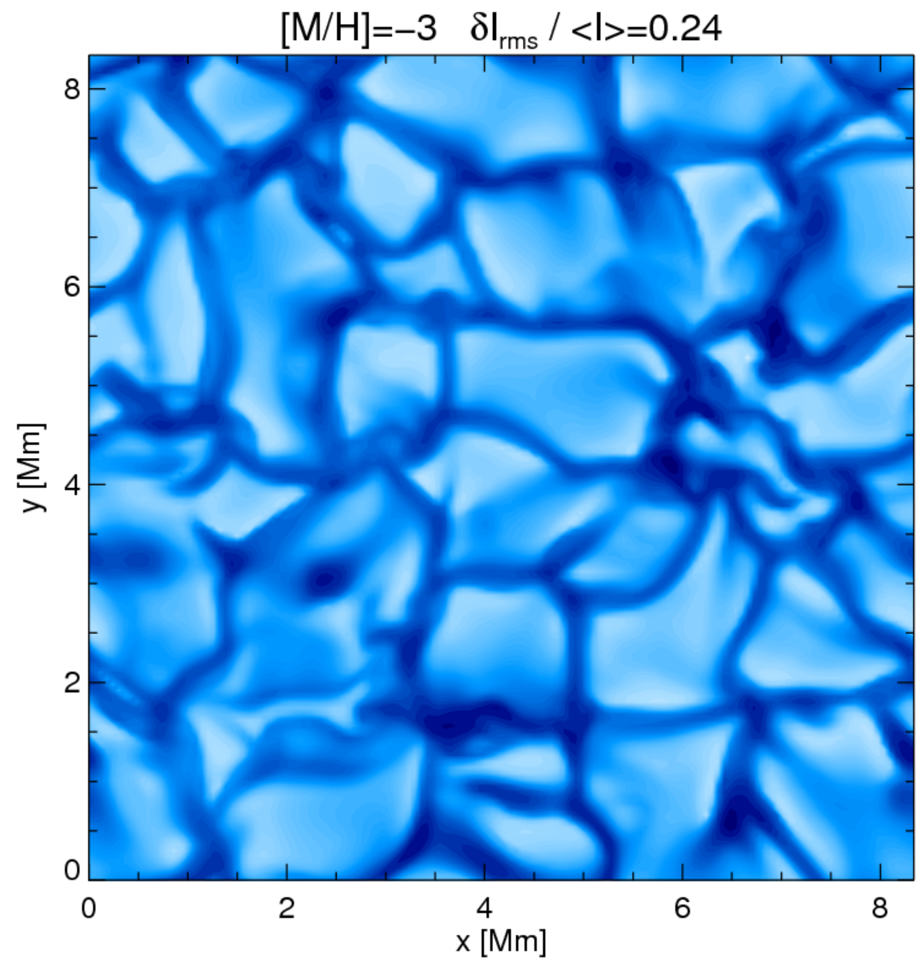
Magnetic field topology HD37776 (aka Landstreet's star)



(©Kochukhov et al. 2010)

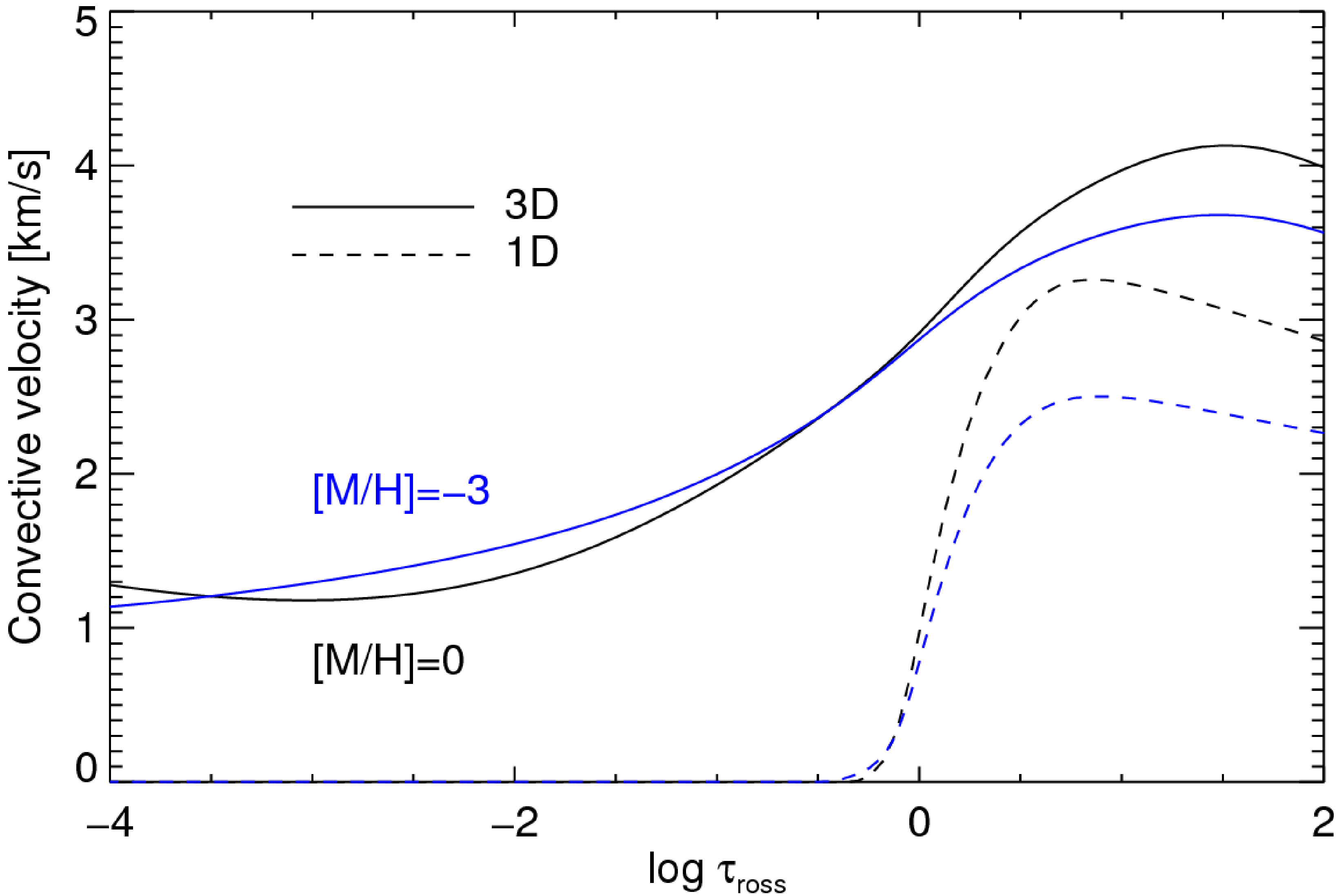
Convection introduces horizontal temperature fluctuations at all metallicities





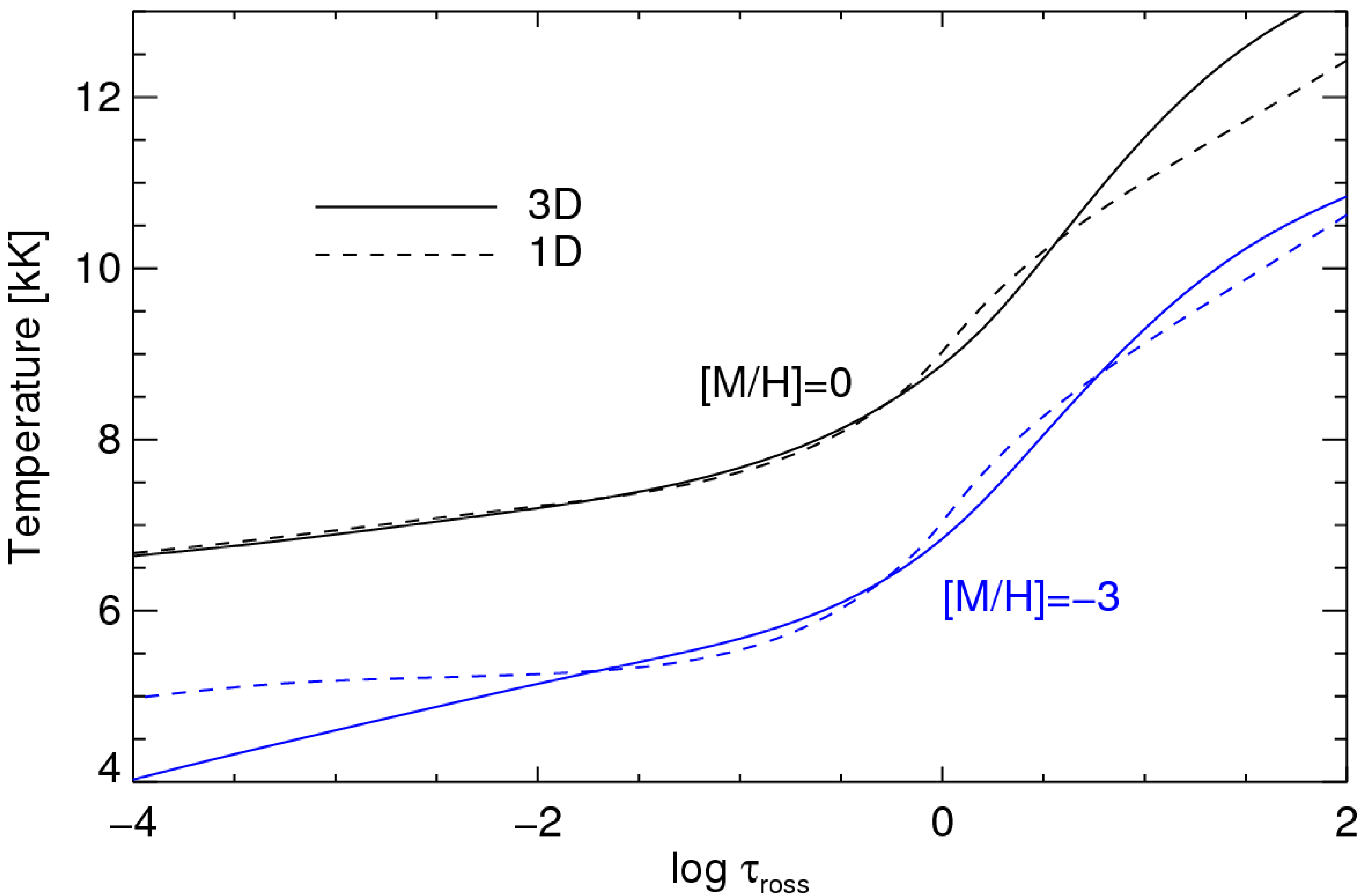
$(T_{\rm eff}{=}6500\,{\rm K},\ \log g{=}4.5)$

Convective overshooting takes place at all metallicities



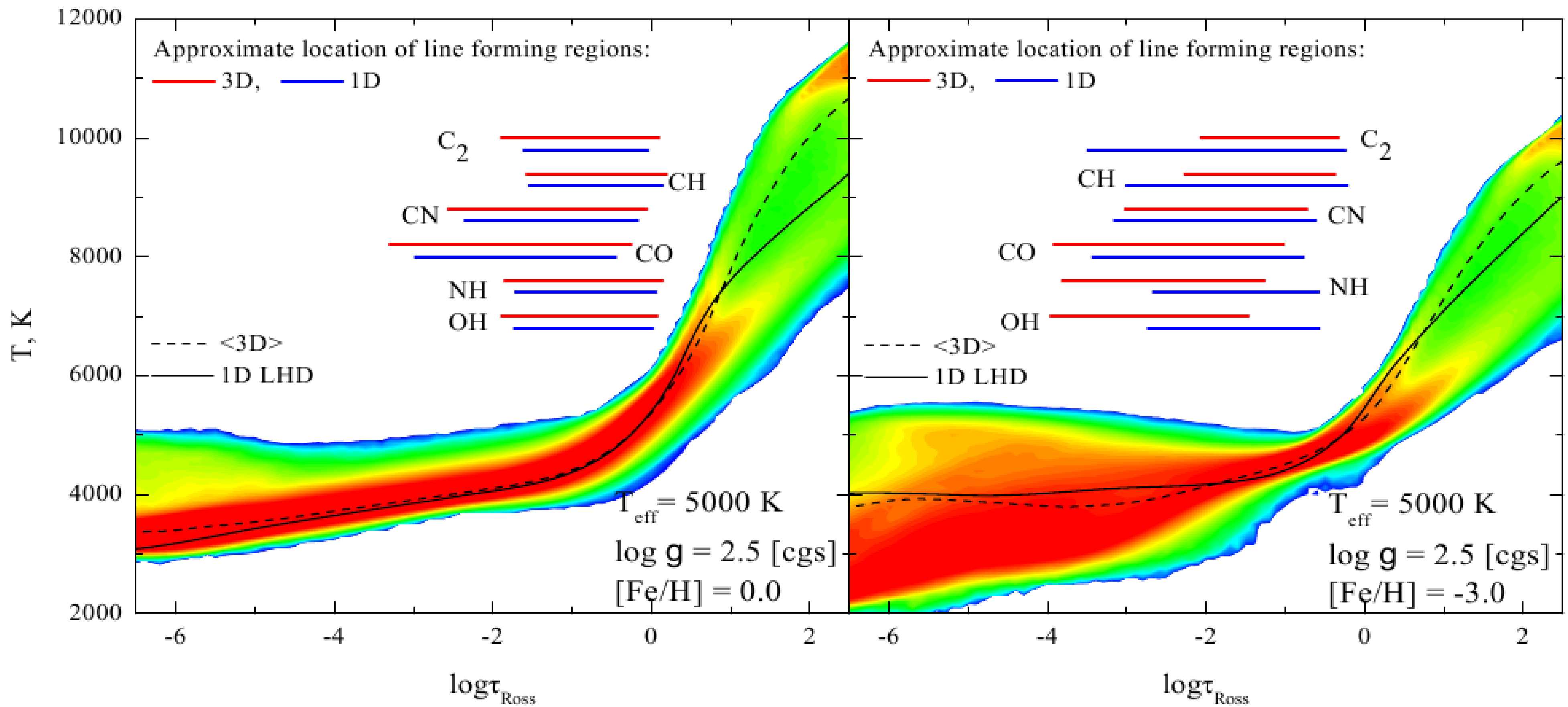
- 3D models predict strong overshooting ($v_{\rm z}^{\rm rms}$) $\rightarrow$ micro/macro-turbulence

Response to convective overshooting depends on metallicity



- Cooling/heating of outer/deeper photospheric layers stronger at low metallicity

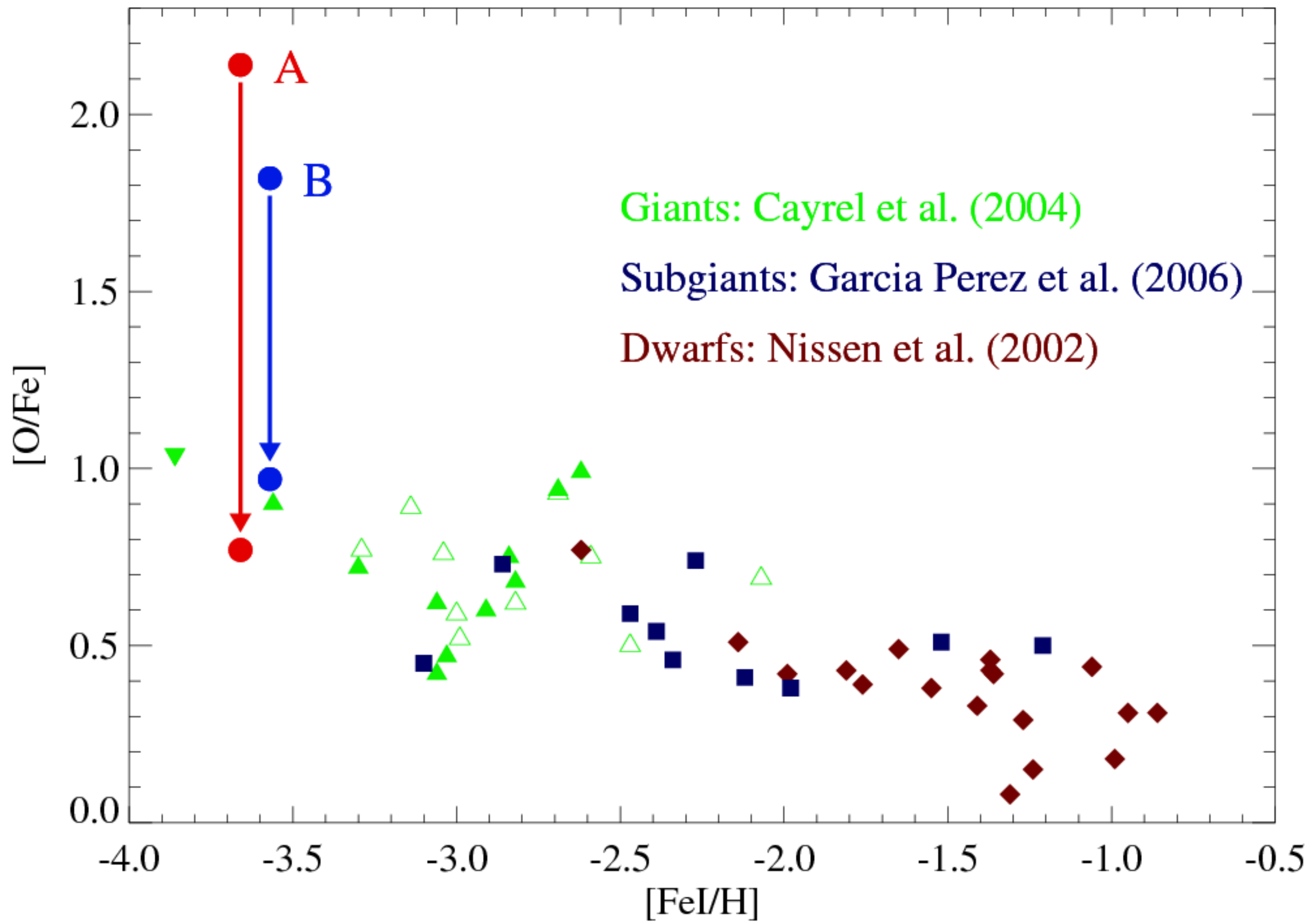
3D effects on RG temperature structure



(from Ivanauskas et al. 2010)

- Two 3D effects on T-structure
  - change of mean temperature with respect to 1D MLT model
  - strong fluctuations around the mean
- Rather modest change of mean structure at rather low metallicity

Binary CS 22876-032 ([Fe/H]≈-3.7): OH vs [OI] 630nm



plot courtesy of J. González Hernández

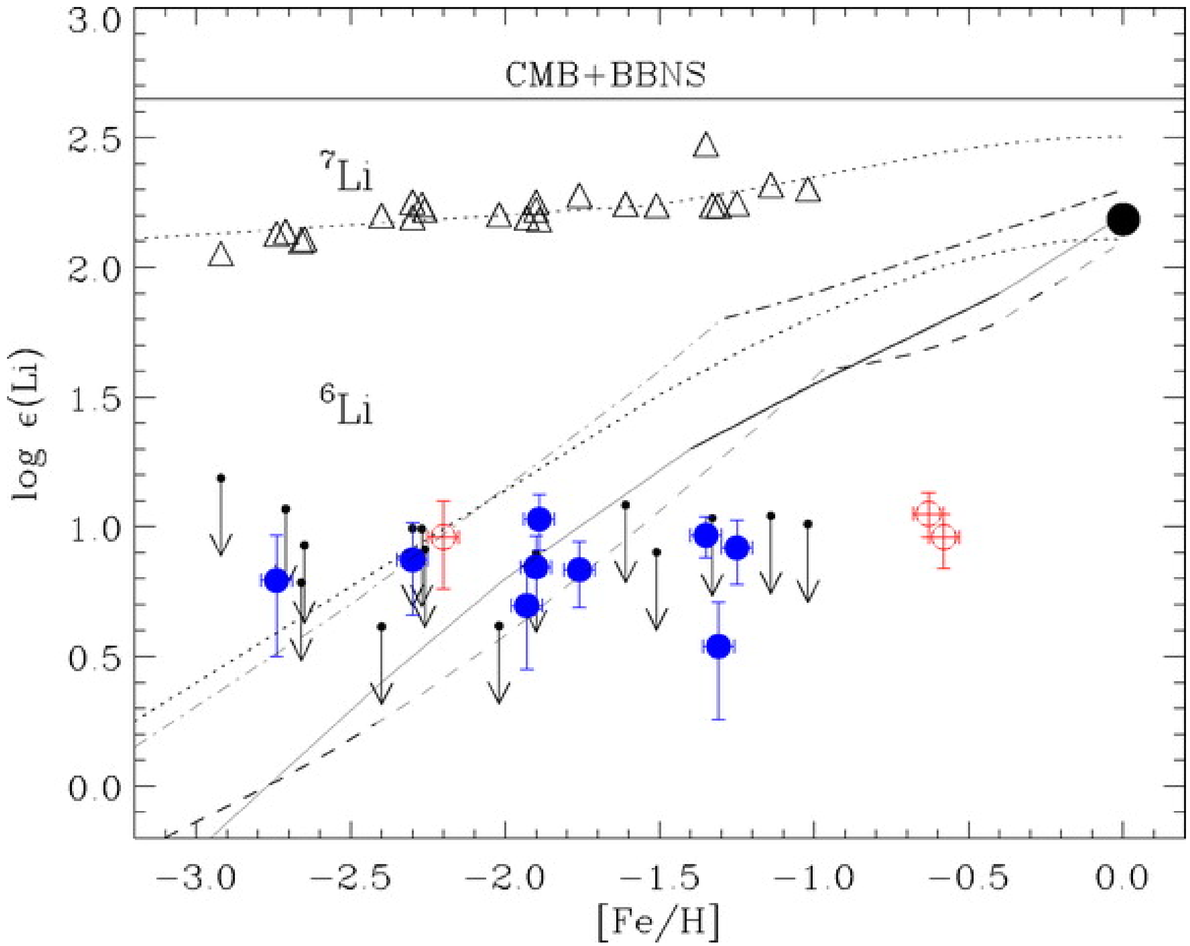
- O abundances from OH lines in the UV, 3D abundance corrections -1.0. . .-1.5 dex
- Binary components (Star A/B) support the notion of a slope in the O/Fe ratio

CO^{5}BOLD **3D abundances (E. Caffau) in comparison to others**

EL	N	CO^{5}BOLD	AG89	GS98	AGS05	AGSS09
Li	1	1.02 ± 0.02	1.16 ± 0.10	1.10 ± 0.10	1.05 ± 0.10	1.05 ± 0.10
C	43	8.50 ± 0.11	8.56 ± 0.04	8.52 ± 0.06	8.39 ± 0.05	8.43 ± 0.05
N	12	7.86 ± 0.12	8.05 ± 0.04	7.92 ± 0.06	7.78 ± 0.06	7.83 ± 0.05
O	10	8.76 ± 0.07	8.93 ± 0.035	8.83 ± 0.06	8.66 ± 0.05	8.69 ± 0.05
P	5	5.46 ± 0.04	5.45 ± 0.04	5.45 ± 0.04	5.36 ± 0.04	5.41 ± 0.03
S	9	7.15 ± 0.06	7.21 ± 0.06	7.33 ± 0.11	7.14 ± 0.05	7.12 ± 0.03
Eu	5	0.52 ± 0.03	0.51 ± 0.08	0.51 ± 0.08	0.52 ± 0.06	0.52 ± 0.04
Hf	4	0.87 ± 0.04	0.88 ± 0.08	0.88 ± 0.08	0.88 ± 0.08	0.85 ± 0.04
Th	1	0.08 ± 0.03	0.12 ± 0.06	$\mathit{0.09 \pm 0.02}$	$\mathit{0.06 \pm 0.05}$	0.02 ± 0.10
K	6	5.10 ± 0.09	5.12 ± 0.13	5.12 ± 0.13	5.08 ± 0.07	5.03 ± 0.09
Fe	15	7.51 ± 0.08	7.67 ± 0.03	7.50 ± 0.05	7.45 ± 0.05	7.50 ± 0.04
Os	3	1.15 ± 0.06	1.45 ± 0.10	1.45 ± 0.10	1.45 ± 0.10	1.25 ± 0.07
Z		0.0154	0.0189	0.0171	0.0122	0.0134
Z/X		0.0211	0.0267	0.0234	0.0165	0.0183

AG89 Anders & Grevesse Geochemica et Cosmochimica acta, 1989 Vol. 53 (6th place)
GS98: Grevesse et Sauval; Space Science Reviews 85: 161-174, 1998
AGS05: Asplund et al.; ASP Conferences Series, Vol. 336, 2205
AGGS09: Asplund, Grevesse, Sauval, & Scott, 2009, ARAA 47, 481

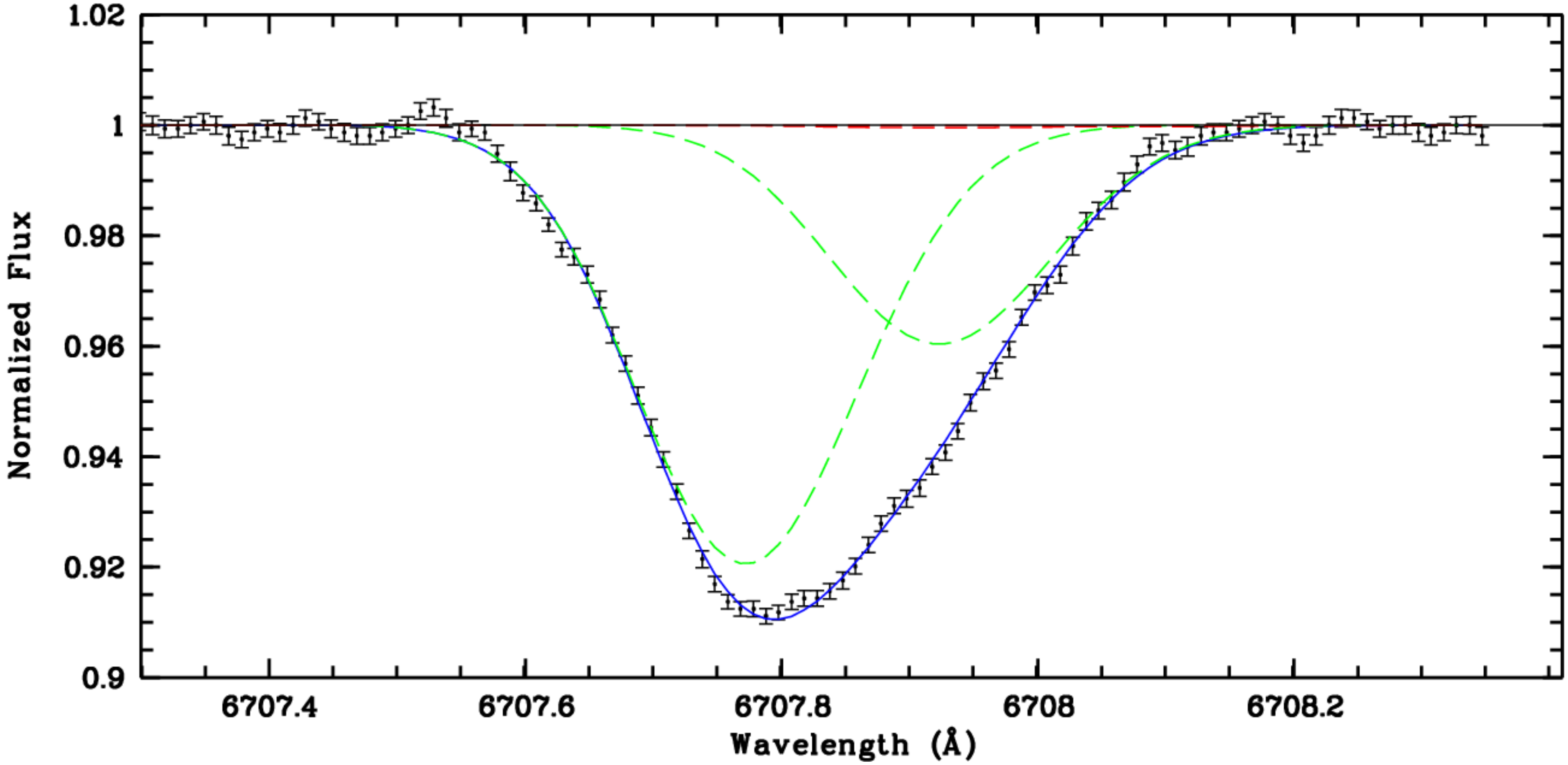
^{6}Li and ^{7}Li in metal-poor halo stars



(Asplund et al. 2006; Smith et al. 1993, 1998; Cayrel et al. 1999; Nissen et al. 1999; chemical evolution models: Prantzos 2006; Ramaty et al. 2000; Fields & Olive 1999; Vangioni-Flam et al. 2000)

- Not corrected for stellar endogenic depletion; arrows indicate 3σ upper limits
- Essentially no ^{6}Li production during Big Bang; but measured isotopic ratio ≈ 0.05

Case study of difficult spectroscopic measurement: ^{6}Li/^{7}Li isotopic ratio in the metal-poor halo dwarf HD74000



- Outstanding observational material: 20h HARPS, $\lambda/\Delta\lambda \approx 110\,000$, $\mathrm{S/N} \approx 600$
- 3D convective line asymmetry and NLTE effects mimic presence of ^{6}Li
- Casts doubts on all previous 1D measurements