Radiative Transfer Methods: New Exact Results (Code ARTY) and Testing the Accuracy of Some Numerical and Approximate Methods (e.g. ALI-like methods)

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Outline

- History
- Survey of methods
- 2 slides of formula (standard problem)
- Known difficulties
- ALI tests
- Exact results: ARTY
- Classical reference solutions and benchmarks
- Test 1: albedo = 0 (cosmology)
- ALI: what's wrong, how to improve ?
- conclusion

History

- Transport theory (TT) : propagation of light (energy) in an absorbing, emitting and scattering medium
- founded par astrophysicists (early 20th) : Schuster (1905), Schwarzschild (1906,1914)
- First reviews: Milne (1930), Hopf (1934)
- TT interdisciplinarity : astrophysics, external geophysics, neutronics, chemistry, biology, etc.
- *bibles* 50-60s (astrophysics): Chandrasekhar (1950), Kourganoff (1952), Sobolev (1963, 1975), Busbridge (1960), Ivanov (1973), Van de Hulst (1980)

- Specific intensity $I(\mathbf{r},t,\mathbf{n},\nu)$: 7 variables (too much)

Solving methods

(Wehrse & Kalkofen 2006, A&A Rev.; I. hubeny; R. Despres; J. Morel)

- **Exact** (known mathematical properties, no discretization): Hopf, Busbridge, Mullikin (Das), Ambartsumian, Sobolev (Danielan), $\sqrt{\varepsilon}$-law (Sobolev 1958), Finite Laplace Transform + ARTY (Chevallier & Rutily, 2005),
- **Simulation**: Monte-Carlo
- **Numerical** (full exact equation, discretized variables): discrete ordinates, S_N, spherical harmonics P_N, F_N method (C. Siewert), Feautrier, variable Eddington factor,
  Ax=b: Λ-iteration (ALI/GS/SOR: XIXe-1986), conjugate gradient (Krylov solver) + preconditioning, CEP (M. Elitzur)…
- **Approximate** (equation or solution) : 1-stream, 2-stream, Eddington, no scattering (albedo = 0), diffusion, moment methods (hydro M1…), escape probability …
- **Type?** Statistical methods, unstructured grids, Fourier transform
- **LITTERATURE:** JQSRT, TTSP mainly.

Transfer theory - The standard problem

$$\forall \nu,\ \mu \frac{\partial I}{\partial \tau}(\tau,\mu) = I(\tau,\mu) - S^*(\tau) - \frac{\varpi(\tau)}{2}\int_{-1}^{1} I(\tau,\mu')\mathrm{d}\mu$$

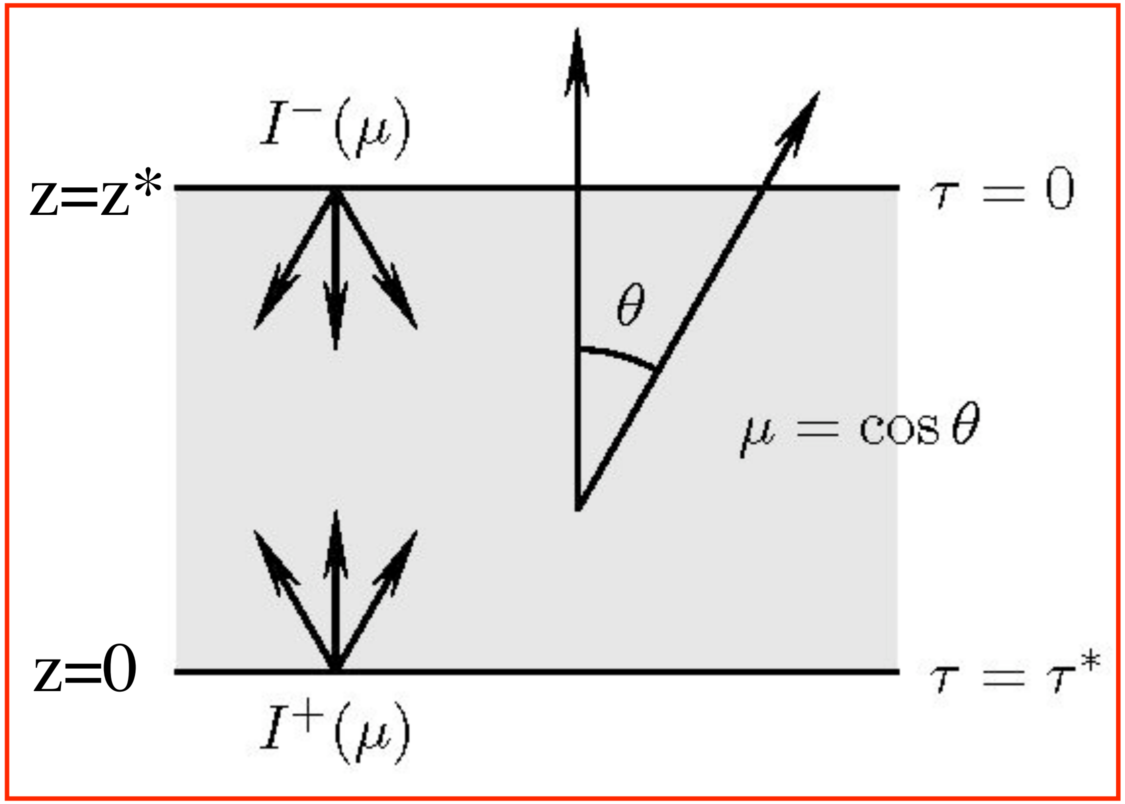
- plane-parallel,
- continuum + line (add ϕ)
- diffusion:
monochromatic, isotropic
- albedo ω = 1 - ε
- S*: internal source (LTE: εB)

$$I_n(\tau) = \frac{1}{2}\int_{-1}^{1} I(\tau,\mu)\mu^n \mathrm{d}\mu$$

$$J(\tau) = I_0(\tau)$$

$$F(\tau) = 4\pi I_1(\tau)$$

$$P(\tau) = \tfrac{4\pi}{c} I_2(\tau)$$



$$\tau = \int_{z}^{z^*} \chi(z')\mathrm{d}z'$$

Transfer theory - integral formulation

(difficulty apparent as compared to differential formulation, and BC)

$$I(\tau,\mu) = \begin{cases} I(0,\mu)\exp(\tau/\mu) - \dfrac{1}{\mu}\displaystyle\int_0^{\tau} S(\tau')\exp\left[(\tau-\tau')/\mu\right]\,\mathrm{d}\tau' & \text{if } -1 \le \mu < 0, \\ S(\tau) & \text{if } \mu = 0, \\ I(\tau^*,\mu)\exp(-(\tau^*-\tau)/\mu) + \dfrac{1}{\mu}\displaystyle\int_{\tau}^{\tau^*} S(\tau')\exp\left[-(\tau'-\tau)/\mu\right]\,\mathrm{d}\tau' & \text{if } 0 < \mu \le +1. \end{cases}$$

$$S(\tau) = [1-\varpi(\tau)]S^*(\tau) + \varpi(\tau)J_0(\tau) + \frac{\varpi(\tau)}{2}\int_0^{\tau^*} E_1(|\tau - t|)S(t)\mathrm{d}t$$

$$J_0(\tau) = \frac{1}{2}\int_{-1}^{0} I^-(\mu)\exp(\tau/\mu)\mathrm{d}\mu + \frac{1}{2}\int_0^1 I^+(\mu)\exp[-(\tau^*-\tau)/\mu]\mathrm{d}\mu$$

- $S = (1-\omega)\, S_0 + \omega\, J$: source function ($J=\Lambda$: mean intensity)
- $S_0 = (1-\omega)\, S^* + \omega\, J_0$: primary source fonction (known)
- LTE: $S^*(t) = B[T(t)]$ (Planck)
- Difficulties due to scattering: $\omega \rightarrow 1$ and/or $\tau^* \rightarrow +\infty$

ALI method - principle

(I. Hubeny, *Stellar Atmospheres Theory: An introduction*, 2001)

In a seminal paper Cannon (1973) introduced into astrophysical radiative transfer theory the *method of deferred corrections* (also called, somewhat inaccurately, an *operator splitting*), long known in numerical analysis. The idea consists of writing

$$\Lambda = \Lambda^* + (\Lambda - \Lambda^*) \ , \tag{121}$$

where Λ^* is an appropriately chosen *approximate lambda operator*. The iteration scheme for solving (119) may then be written as

$$S^{(n+1)} = (1-\epsilon)\Lambda^*[S^{(n+1)}] + (1-\epsilon)(\Lambda - \Lambda^*)[S^{(n)}] + \epsilon B \ , \tag{122}$$

or, in a slightly different form whose importance becomes apparent later,

$$S^{(n+1)} - S^{(n)} = [1 - (1-\epsilon)\Lambda^*]^{-1}[S^{\rm FS} - S^{(n)}] \ , \tag{123}$$

where

$$S^{\rm FS} = (1-\epsilon)\Lambda[S^{(n)}] + \epsilon B \ . \tag{124}$$

Known difficulties (solutions)

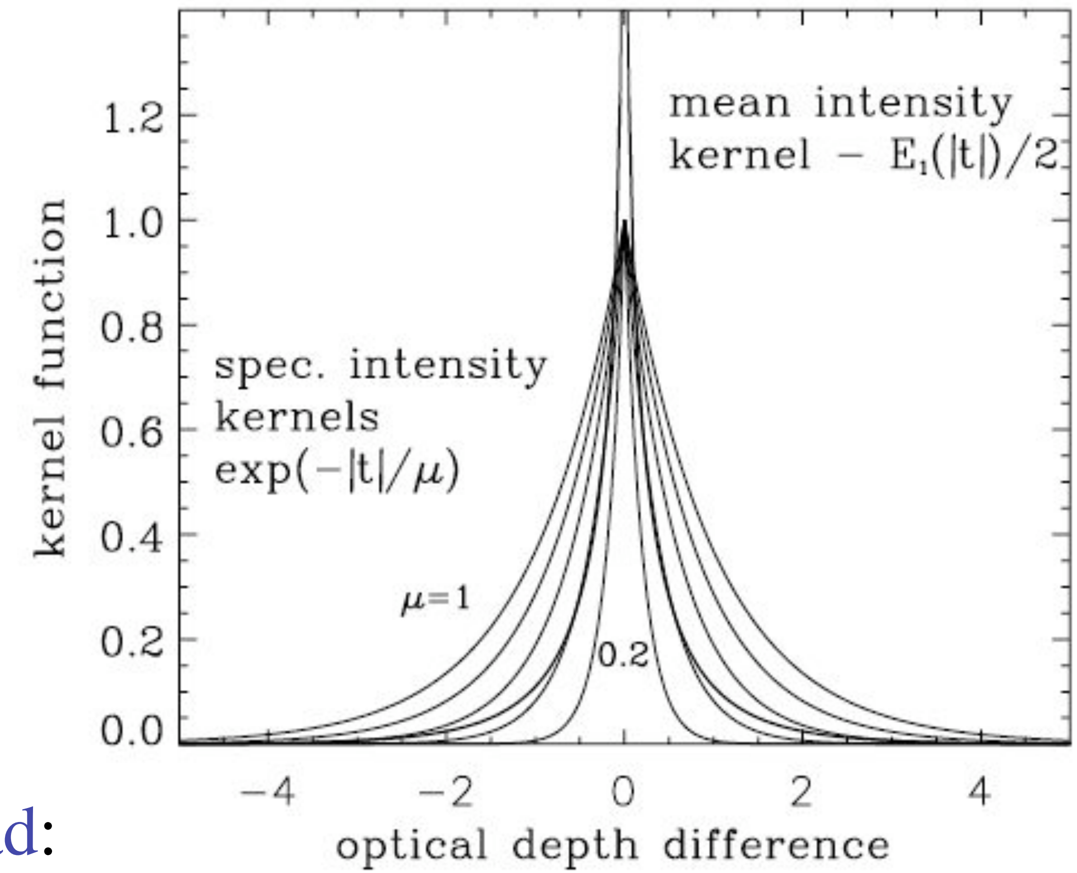
$$S(\tau) = S_0(\tau) + \varpi(\tau)\frac{1}{2}\int_0^{\tau^*} E_1(|t-\tau|)S(t)dt$$

- E_1 narrow: slow convergence (preconditioning, acceleration)
- E_1 weakly singular: $dS/d\tau(0)$ infinite (grid refinement)
- (High) gradients in S_0 (gr, linear interpolation instead parabolic)
- Optically thick spectral lines ($\tau^* >> 1$, $1-\omega << 1$) (gr)
- Iterative methods stopping criterion (multi-grid?)
- Discretization, numerical parameters (gr), roundoff errors
- Iterative methods are slow, e.g. multi-D (Krylov, parallel?)

Known difficulties - singular E_1 kernel

$$S(\tau) = S_0(\tau) + \varpi(\tau)\frac{1}{2}\int_0^{\tau^*} E_1(|t-\tau|)S(t)dt$$

$$E_1(\tau) = \int_0^1 \exp(-\tau/\mu)\frac{\mathrm{d}\mu}{\mu}$$



- $E_1(\tau)$: kernel, $E_1(0) = \infty$

➔singular integral equation

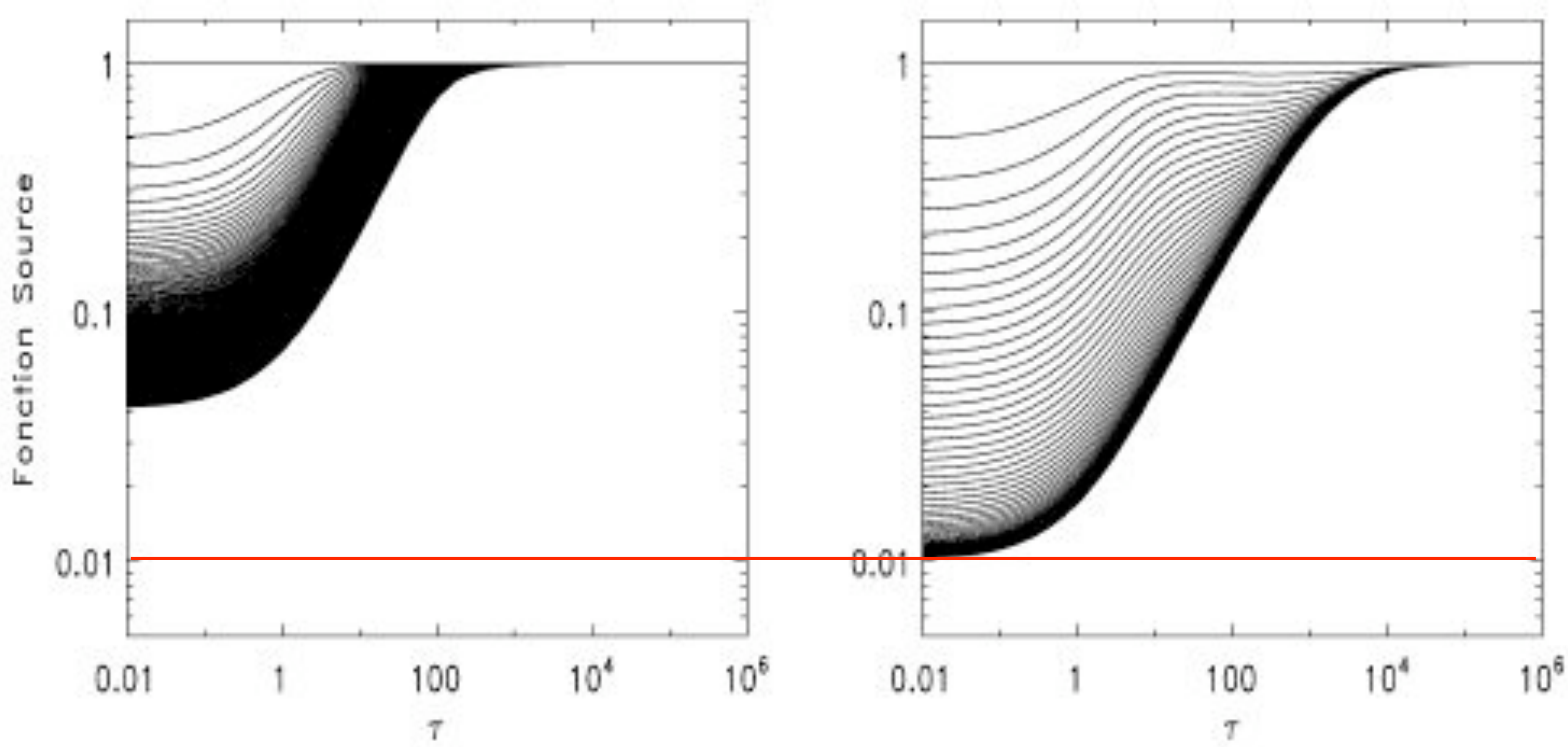
- non-local in τ, but E_1 tiny range,

Ax=b, A almost diagonal

➔ slow convergence

- Escape probability for lines is bad:
  - x2: Hubeny 2001,
  - 50%: Elitzur & Asensio Ramos 2005)

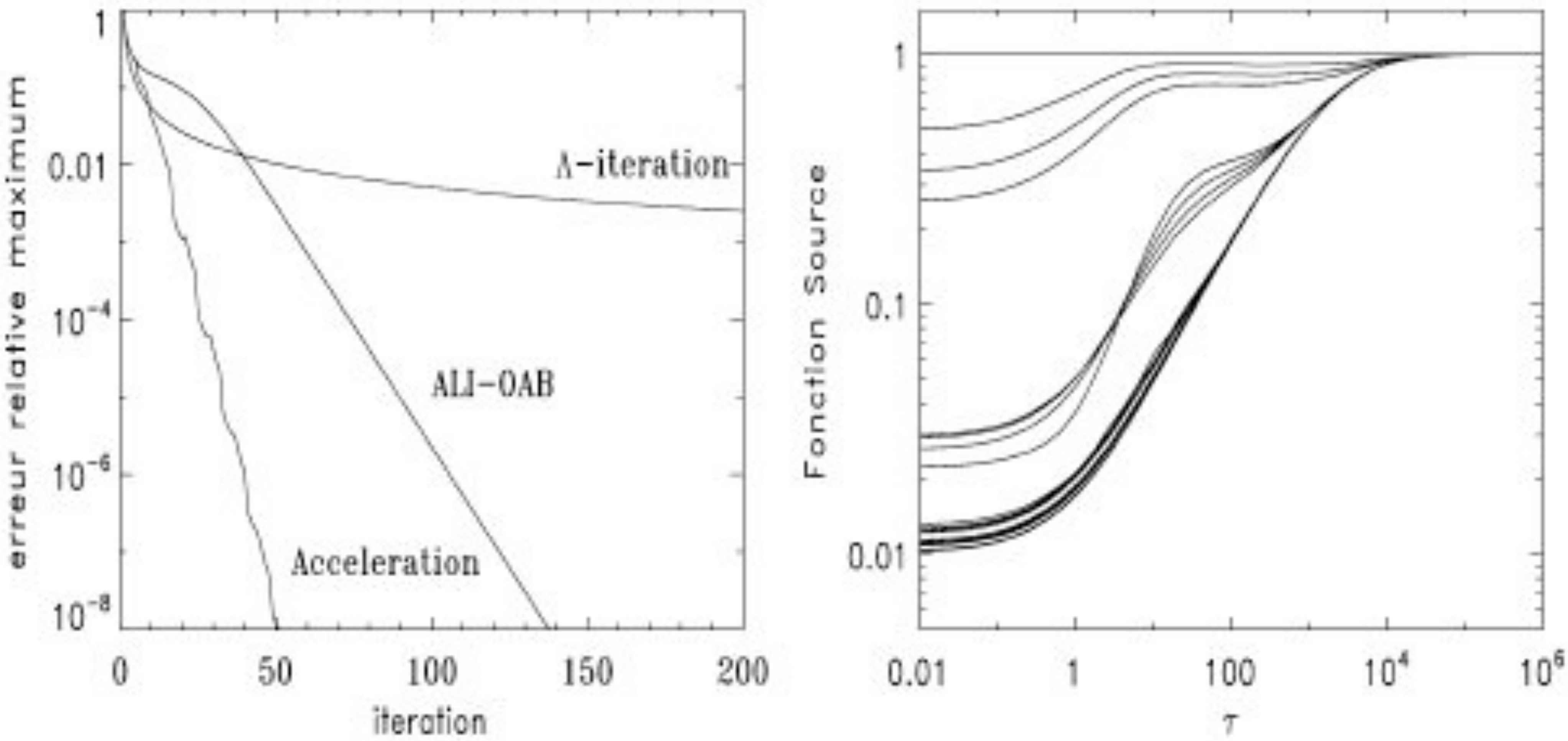
Known difficulties - slow convergence



Source function S(τ) with iterations for Λ-iteration (left) and ALI (right)

Paletou, C. R. Acad. Sci. Paris, t. 2, Serie IV (2001)

Known difficulties - slow convergence



Accuracy with iteration (left) and S(τ) with iterations for ALI+Ng (right)

Paletou, C. R. Acad. Sci. Paris, t. 2, Serie IV (2001)

Known difficulties (solutions)

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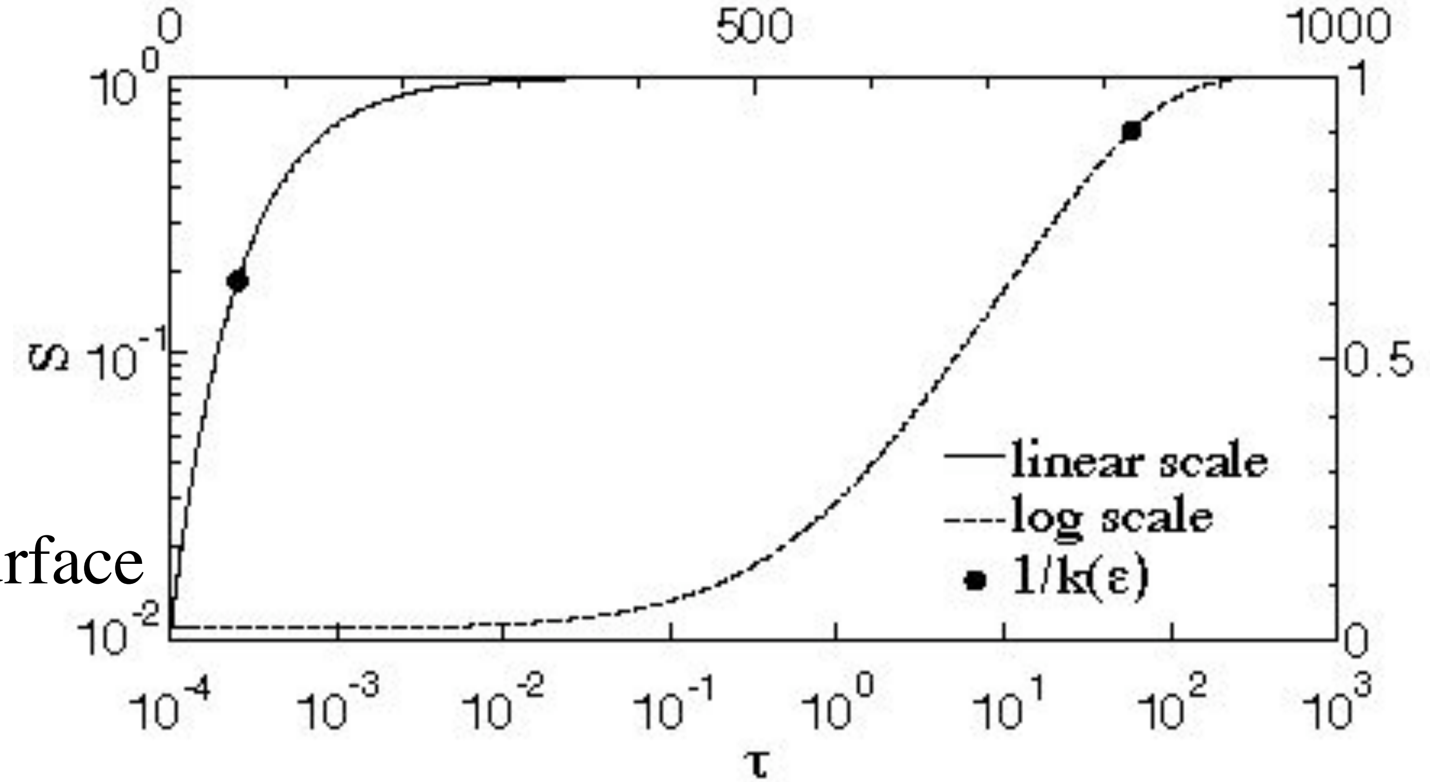
- Optically thick spectral lines ($\tau^* \gg 1$, $1-\omega \ll 1$) (gr)
- Iterative methods stopping criterion (multi-grid?)
- Discretization, numerical parameters (gr), roundoff errors
- Iterative methods are slow, e.g. multi-D (Krylov, parallel?)

Known difficulties - Surface (∞)

$$S(\tau) = S_0(\tau) + \varpi(\tau)\frac{1}{2}\int_0^{\tau^*} E_1(|t-\tau|)S(t)dt$$

- std problem ($S_0=\varepsilon$):
$S(0)=\sqrt{\varepsilon}$, $S(\infty)=1$

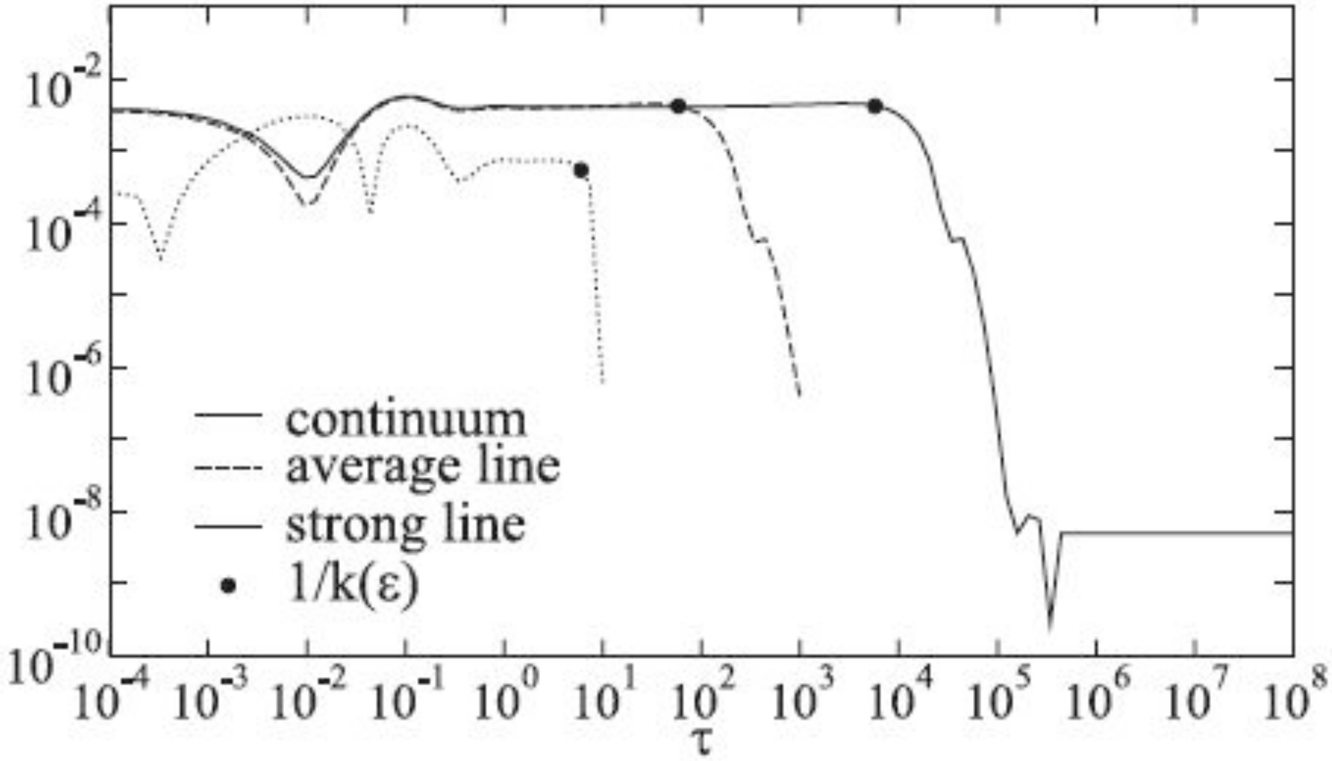
- $dS/d\tau(0)$ infinite
➔ refined grid near surface



Source function S for the standard problem (weak line)
Chevallier, Paletou & Rutily, A&A (2003)

Known difficulties - Surface

• 1-ω, τ^* =
0.5, 2 (continuum),
1e-2, 20 (average line),
1e-8, 2e8 (strong line).
• accuracy worst NEAR surface (grid 1e-4)
• needs refined grid near surface (log-spaced)



Accuracy of ALI for the standard problem
Chevallier, Paletou & Rutily, A&A (2003)

Known difficulties (solutions)

$$S(\tau) = S_0(\tau) + \varpi(\tau)\frac{1}{2}\int_0^{\tau^*} E_1(|t-\tau|)S(t)dt$$

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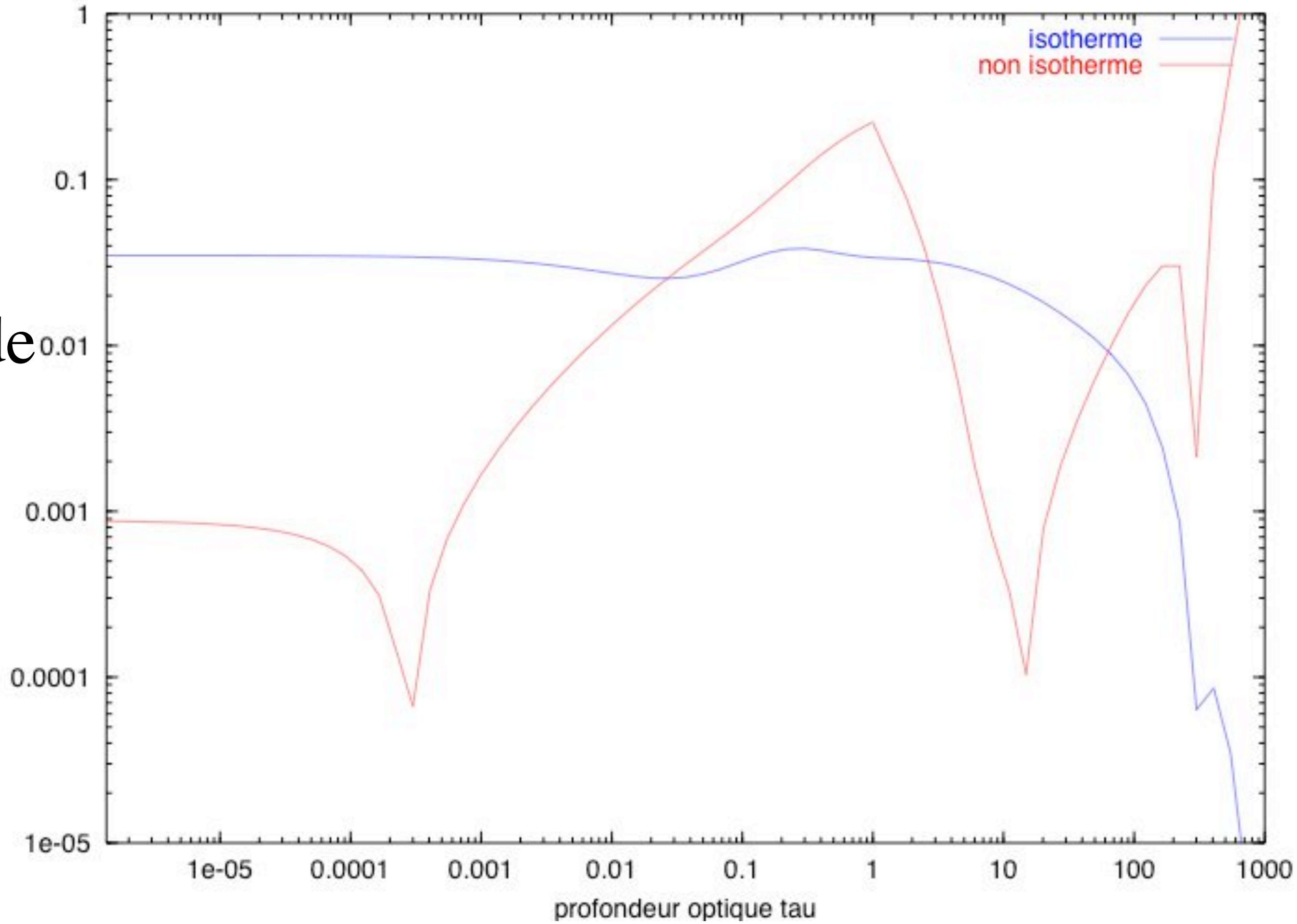
Known difficulties - S_0 gradients

S0 = constant:
4% surface, <<1 inside
S0 = gradient:
0.1% surface, 30% inside
+ roundoff error (small)



ALI accuracy, stellar atmospheres grid
S0 = 1, exp(-τ)

Known difficulties - High S_0 gradients (AGN, P=cte ➔ thermal instability)

- ALI+Ng for transfer
- 600 layers

(50-100/dec. vs. 7 atm.)

Need time (iterations)

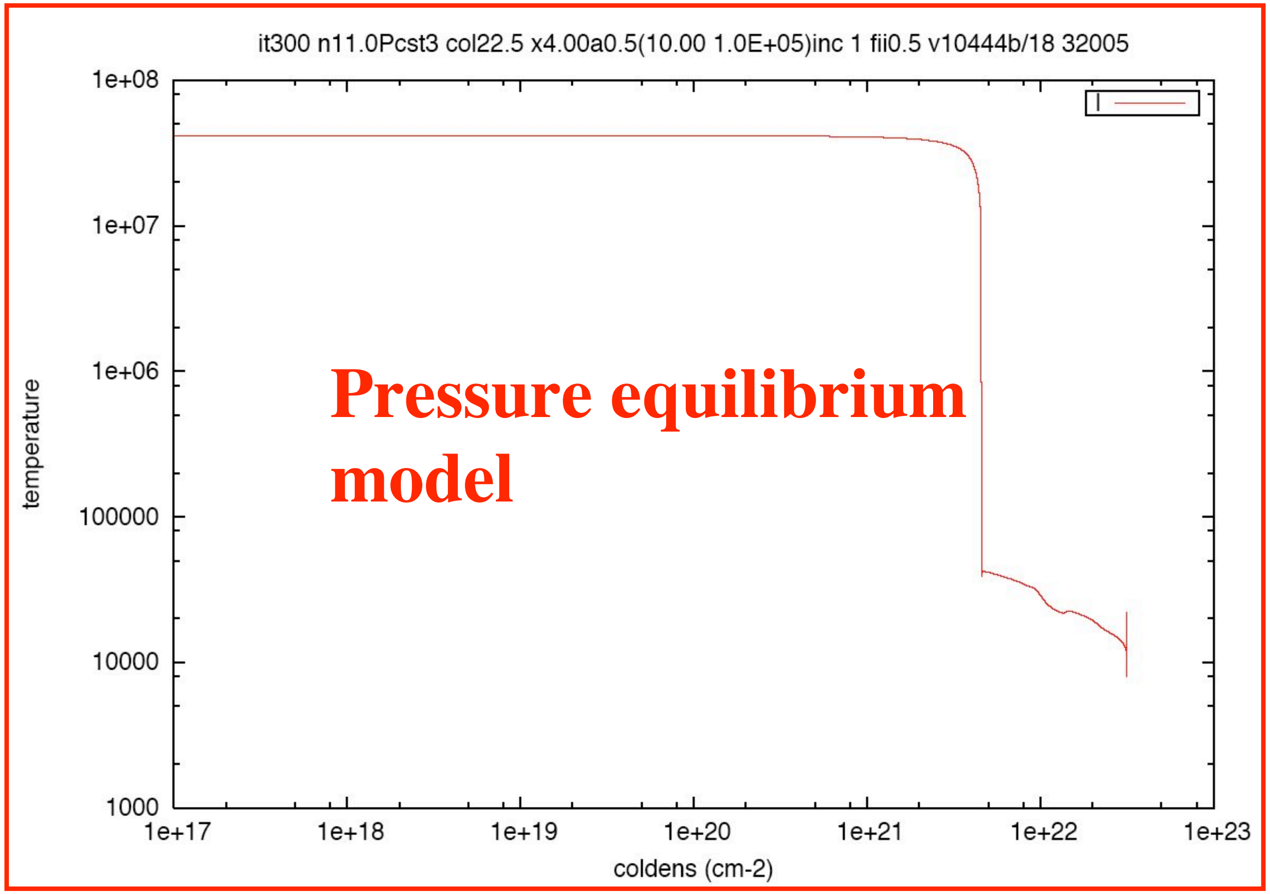
- High gradients

OK : adaptive grid

- Number of angles

OK : choice 3 (vs. 20)

Temperature



Geometrical depth (column density cm-2)

Known difficulties - High S_0 gradients (AGN, P=cte ➔ thermal instability)

- stopping criterium change < 0.1% and less than 100 iterations + empirical convergence tricks
- default : parabolic

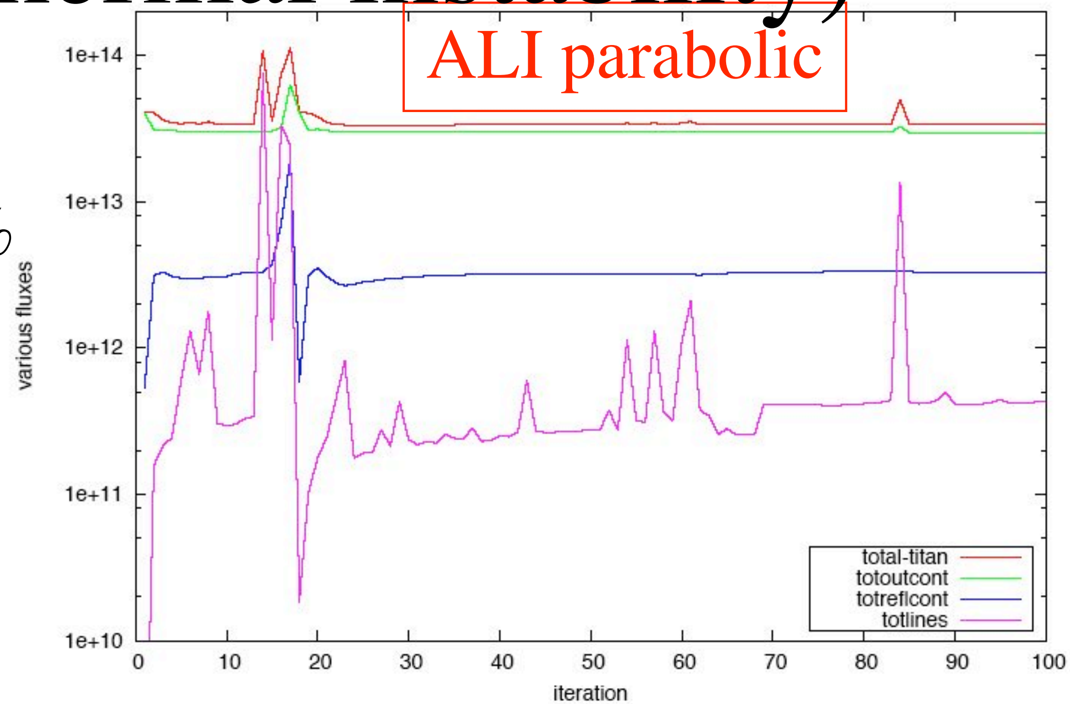
no convergence (some P cte WA)

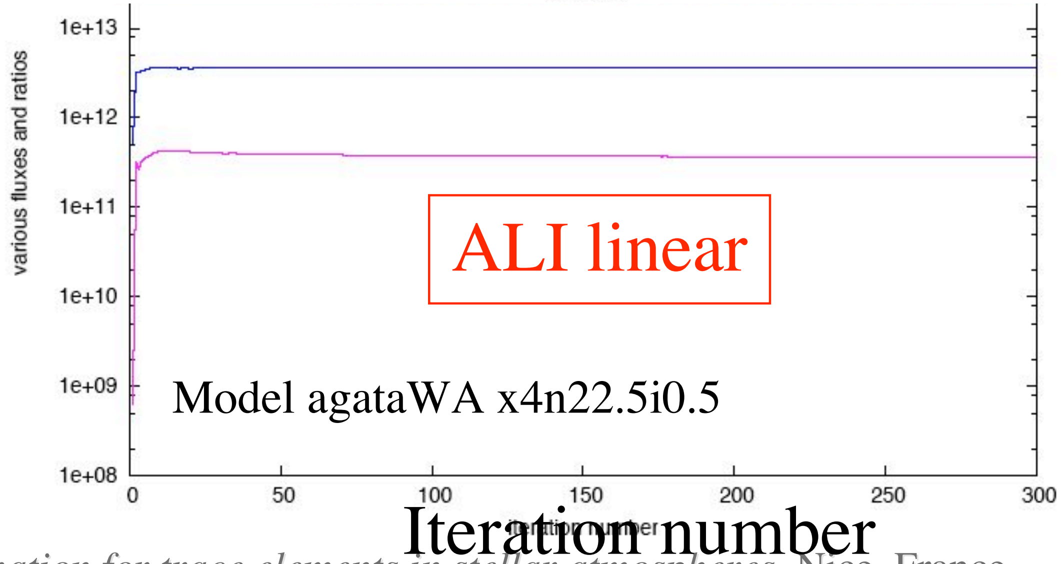
Cause : interpolation instabilities

- 1 solution : linear interpolation

Convergence (not always)

Longer (iterations 300 vs.50)





Known difficulties (solutions)

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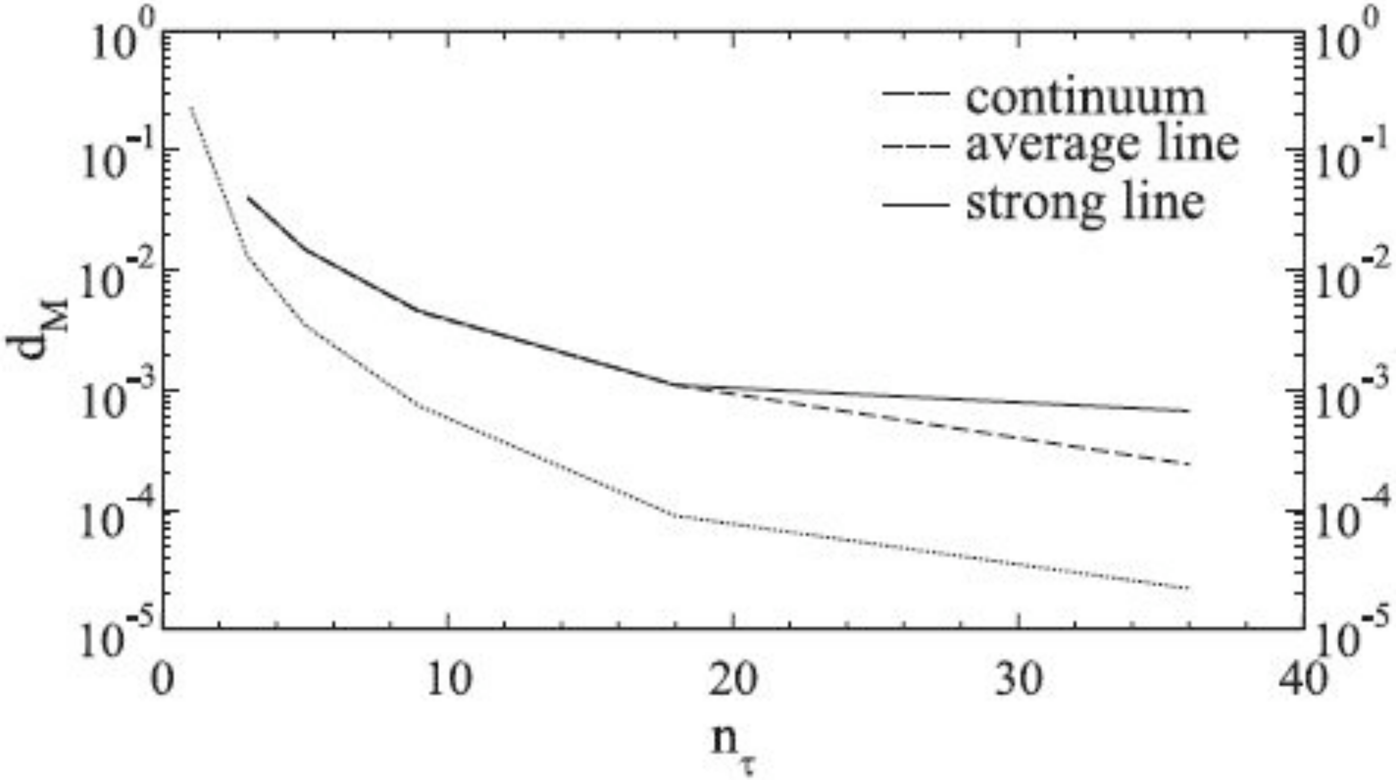
- Discretization, numerical parameters (gr), roundoff errors
- Iterative methods are slow, e.g. multi-D (Krylov, parallel?)

Known difficulties - Discretization
(standard problem)

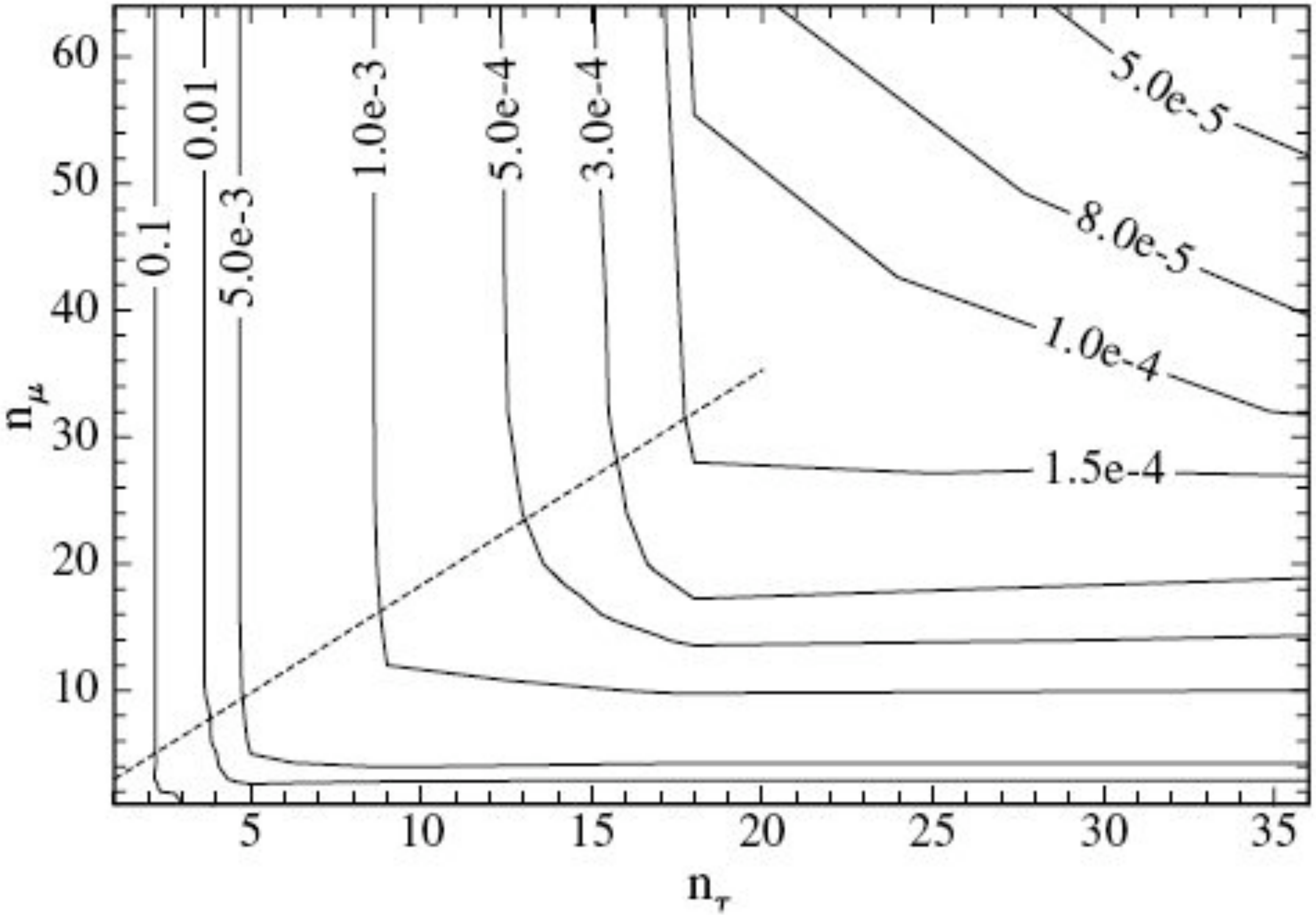
- $1-\omega$, $\tau^* =$
0.5, 2 (continuum),
1e-2, 20 (average line),
1e-8, 2e8 (strong line).
- Maximum error



Accuracy of ALI for the standard problem
Chevallier, Paletou & Rutily, A&A (2003)

Known difficulties - Discretization
(standard problem)

- $1-\omega$, $\tau^* = 1e\text{-}8, 2e8$ (strong line).

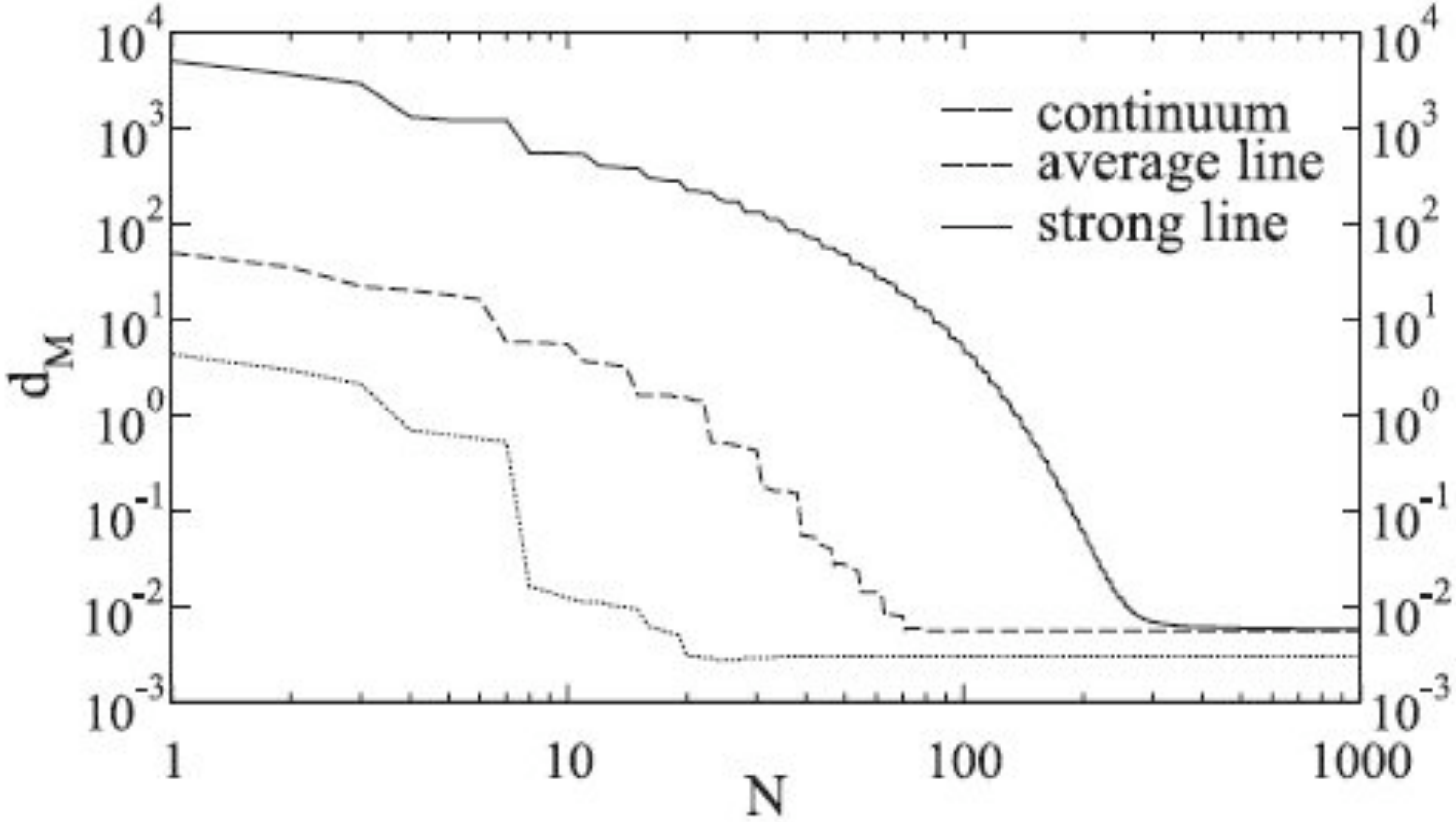


Accuracy of ALI for the standard problem strong line, x=spatial, y=angular

Chevallier, Paletou & Rutily, A&A (2003)

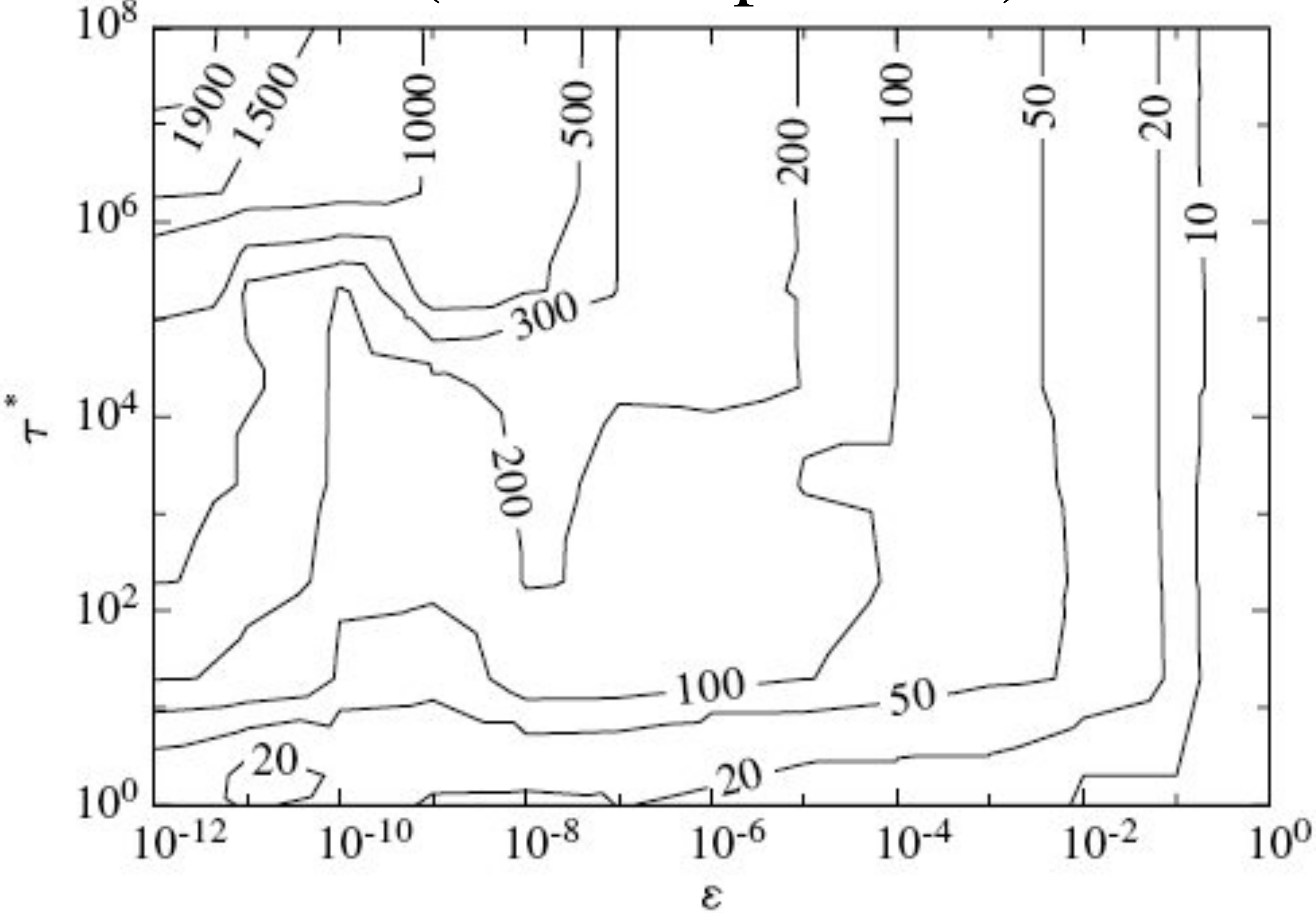
Known difficulties - Discretization
(standard problem)

- 1-ω, τ* =
0.5, 2 (continuum),
1e-2, 20 (average line)
1e-8, 2e8 (strong line)
- Maximum error



Accuracy of ALI for the standard problem
along the iteration number
Chevallier, Paletou & Rutily, A&A (2003)

Known difficulties - Discretization
(standard problem)



Optimal number of iterations of ALI for the standard problem

Chevallier, Paletou & Rutily, A&A (2003)

Known difficulties (solutions)

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- Iterative methods stopping criterion (multi-grid?)
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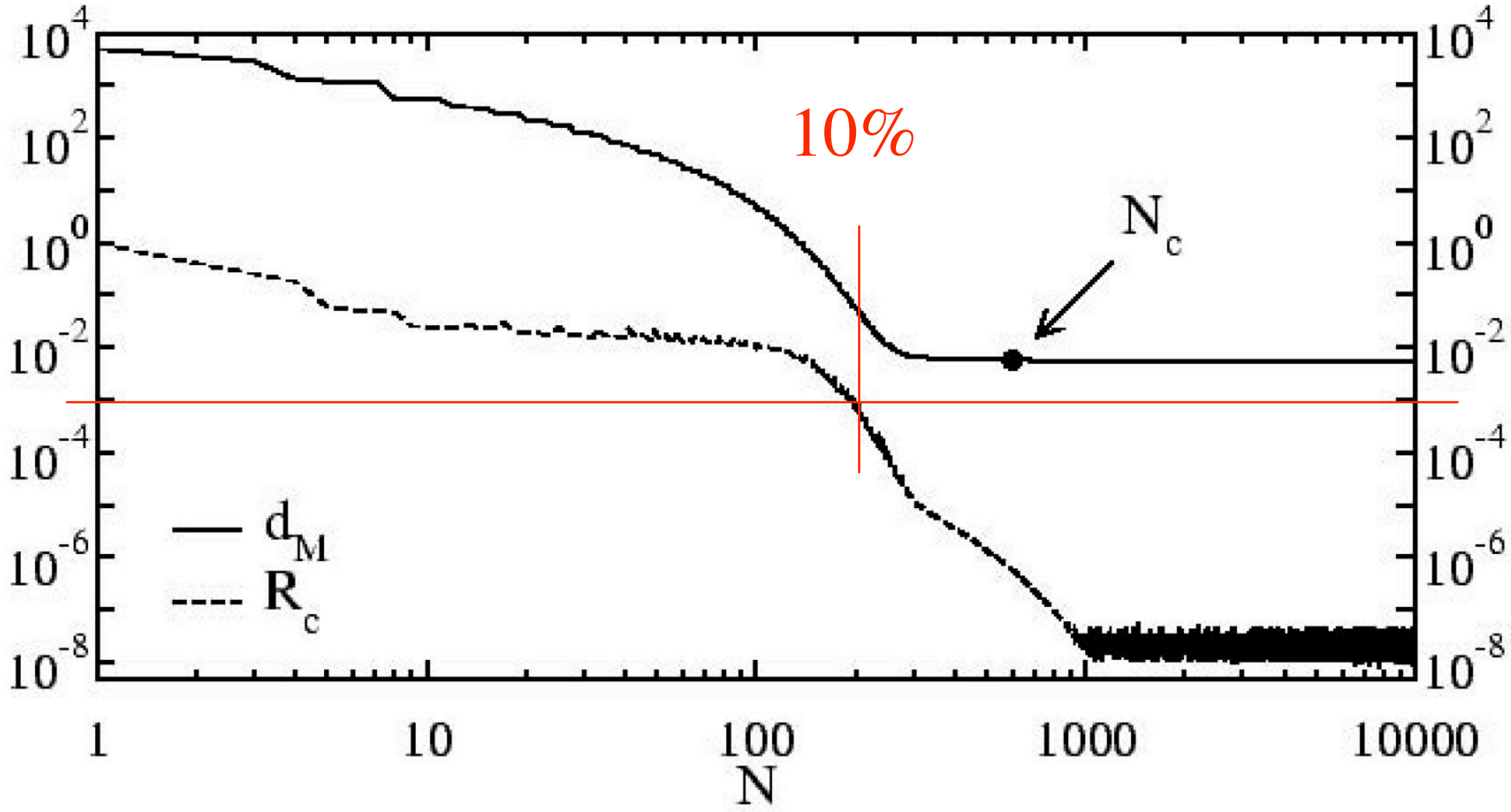
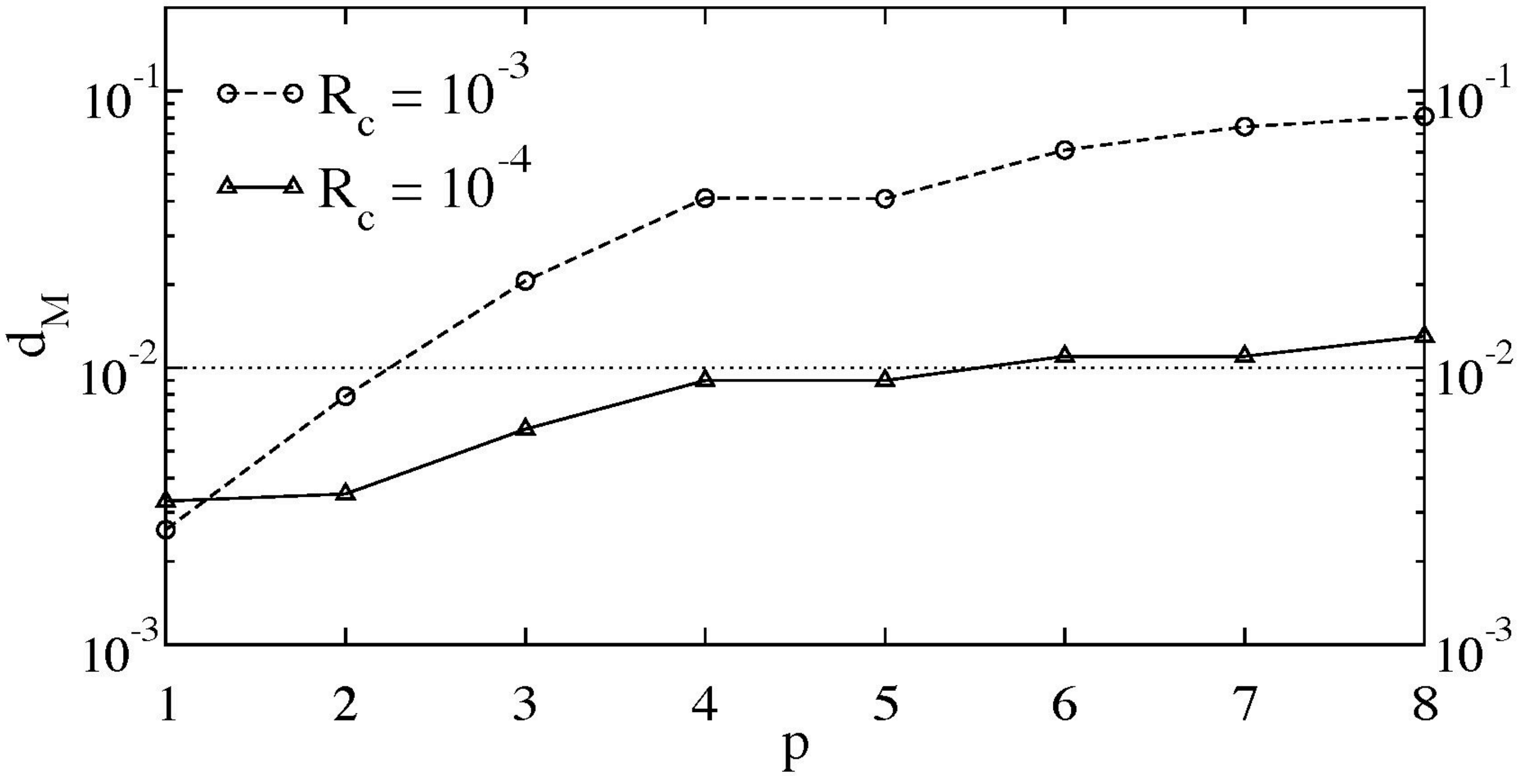
- Iterative methods are slow, e.g. multi-D (Krylov, parallel?)

Known difficulties - Stopping criterion



Accuracy of ALI+Ng for the standard problem with iterations (strong line)
Chevallier, Paletou, & Rutily, SF2A proceedings (2003)

Known difficulties - Stopping criterion

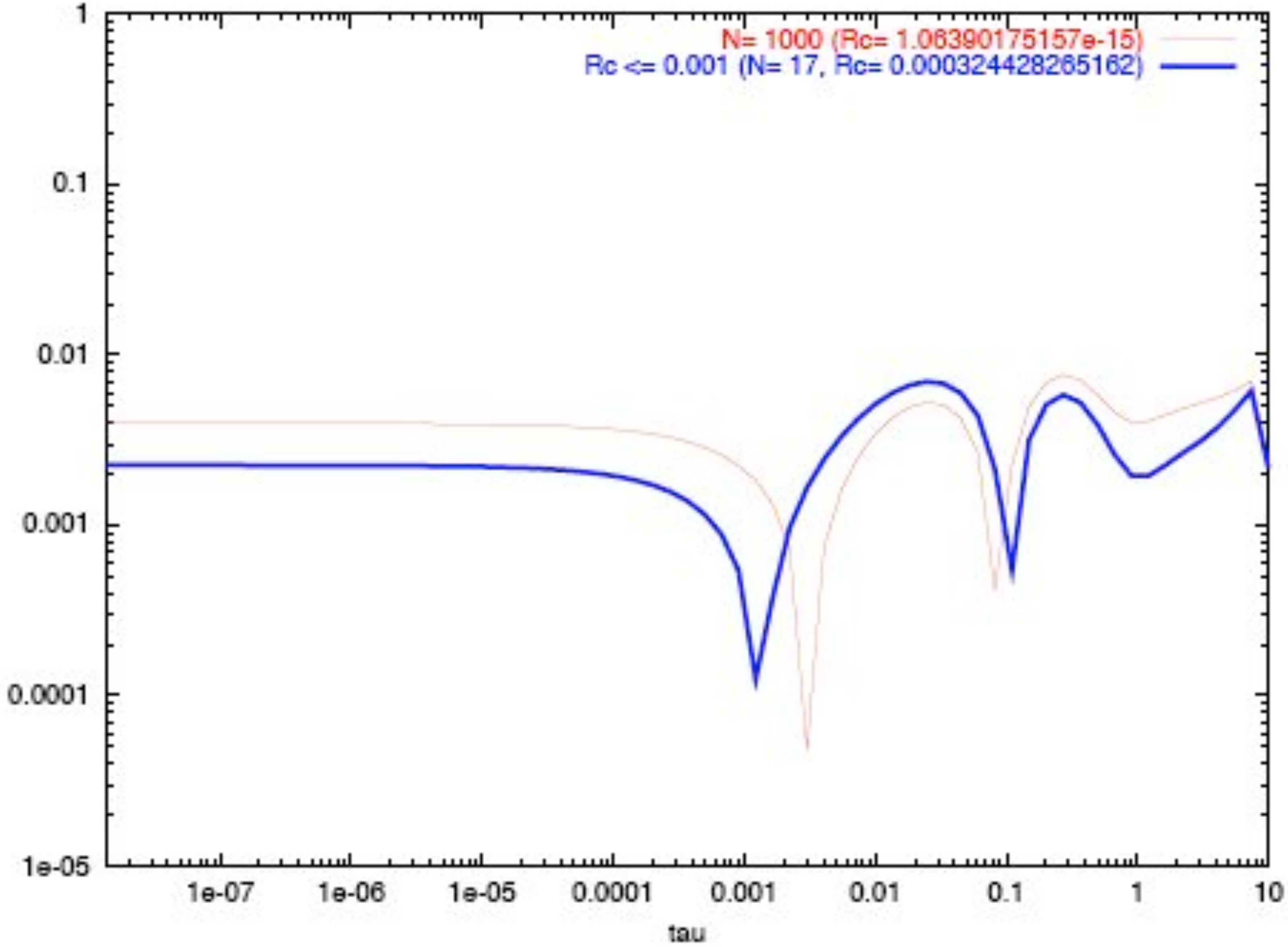


Accuracy of ALI+Ng for the standard problem with difficulty
Chevallier, Paletou, & Rutily, SF2A proceedings (2003)

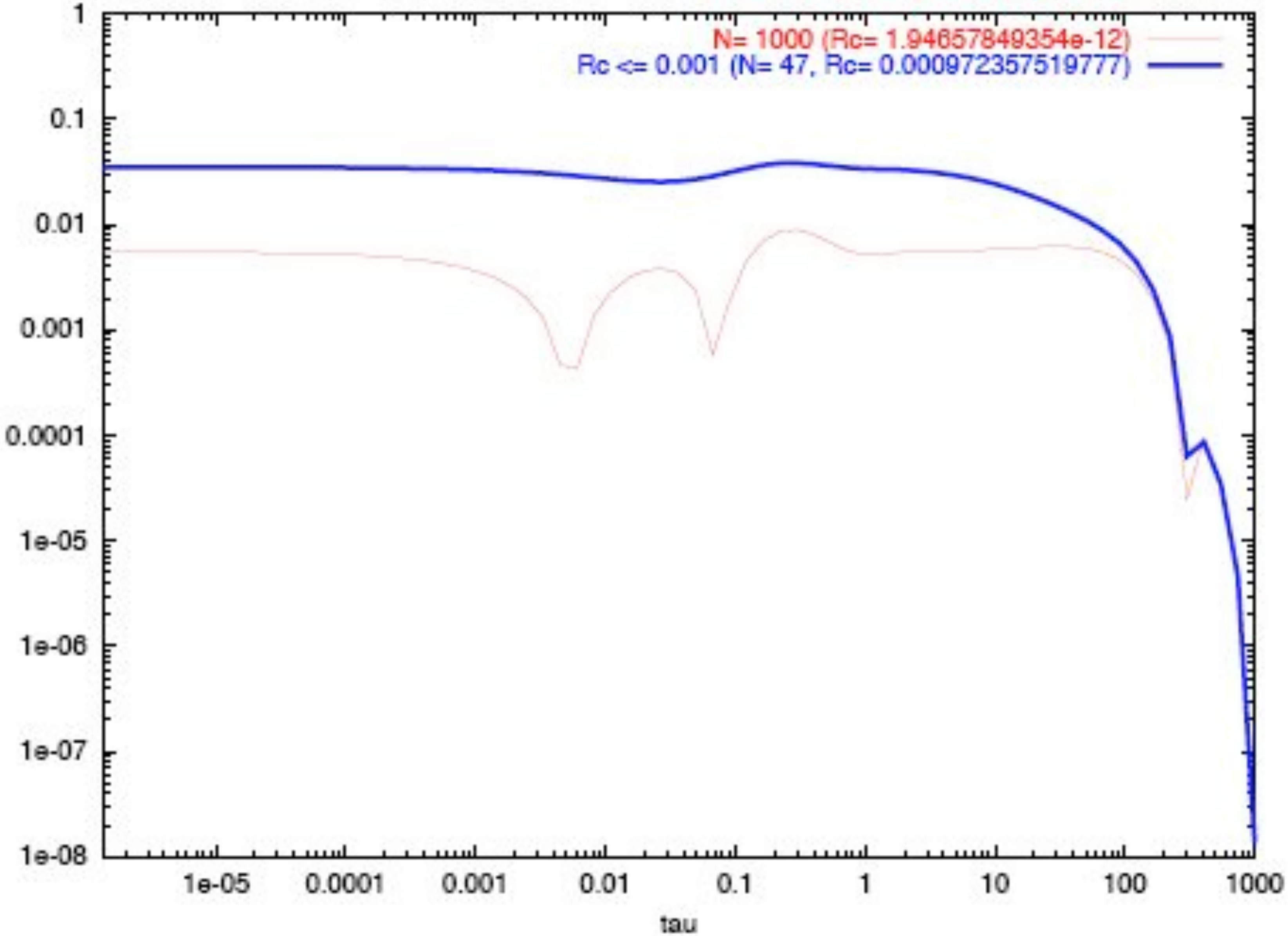
Testing ALI std parameters

- TLUSTY stellar atmosphere code (I. Hubeny) standard parameters
- continuum transfer equation, but equivalent to line also (Milne)
- 4 functions $S0(\tau) = 1, \tau, \tau^5, \exp(-\tau), \exp(\tau)$
- constant albedo ω
- 3 physical conditions $(\omega, \tau^*) =$
  - (0.01,10): continuum,
  - $(10^{-4}, 10^3)$: average line,
  - $(10^{-8}, 10^8)$: strong line.
- logarithmic spatial grid, 70 points from $10^{-9}\,\tau^*$ to τ^*
- Gauss-Legendre angular grid, 3 points per quadrant
- Stop iterations when $R_c = 10^{-3}$.

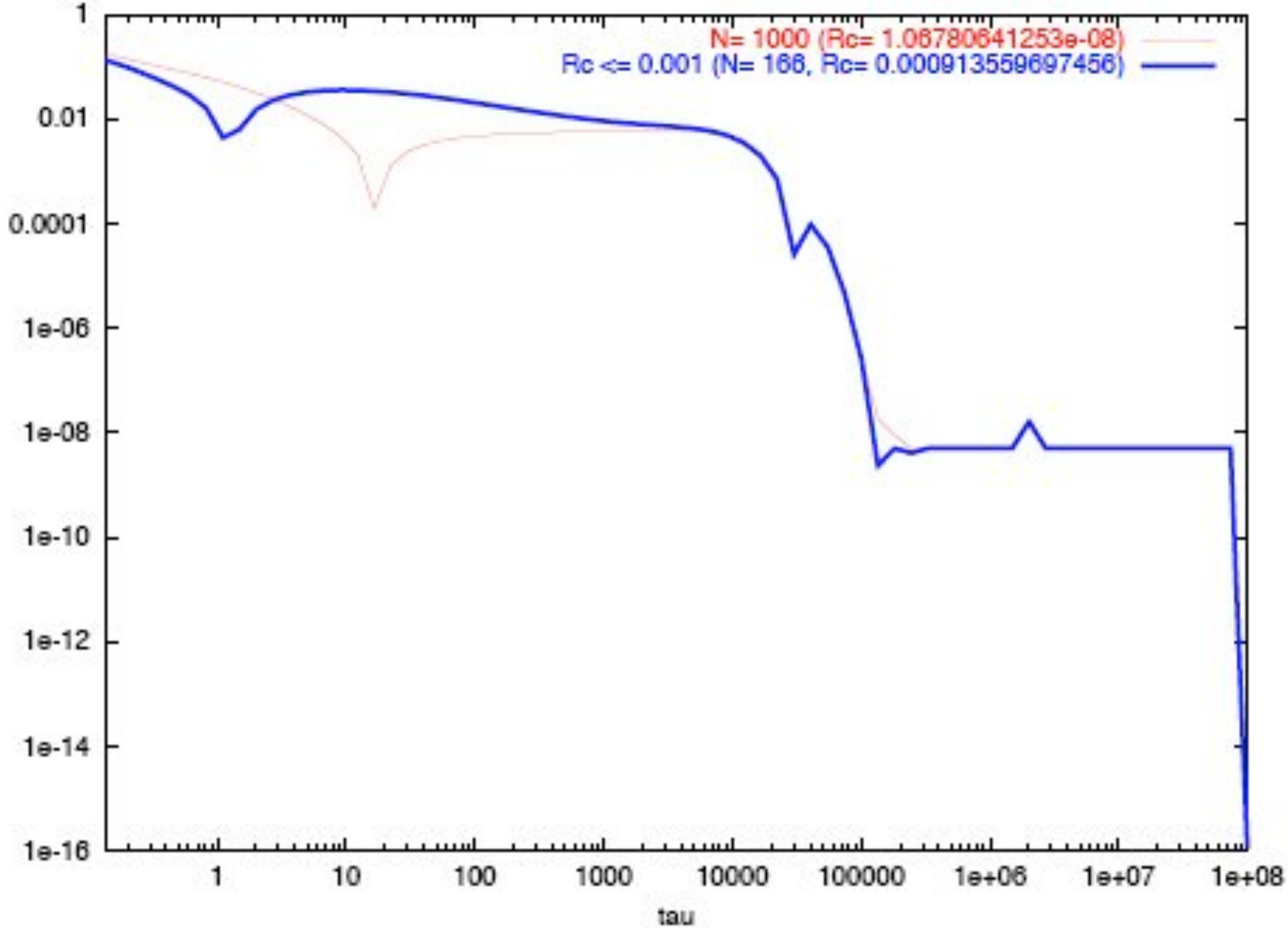
Testing ALI std parameters - B(τ) = 1 (continuum)



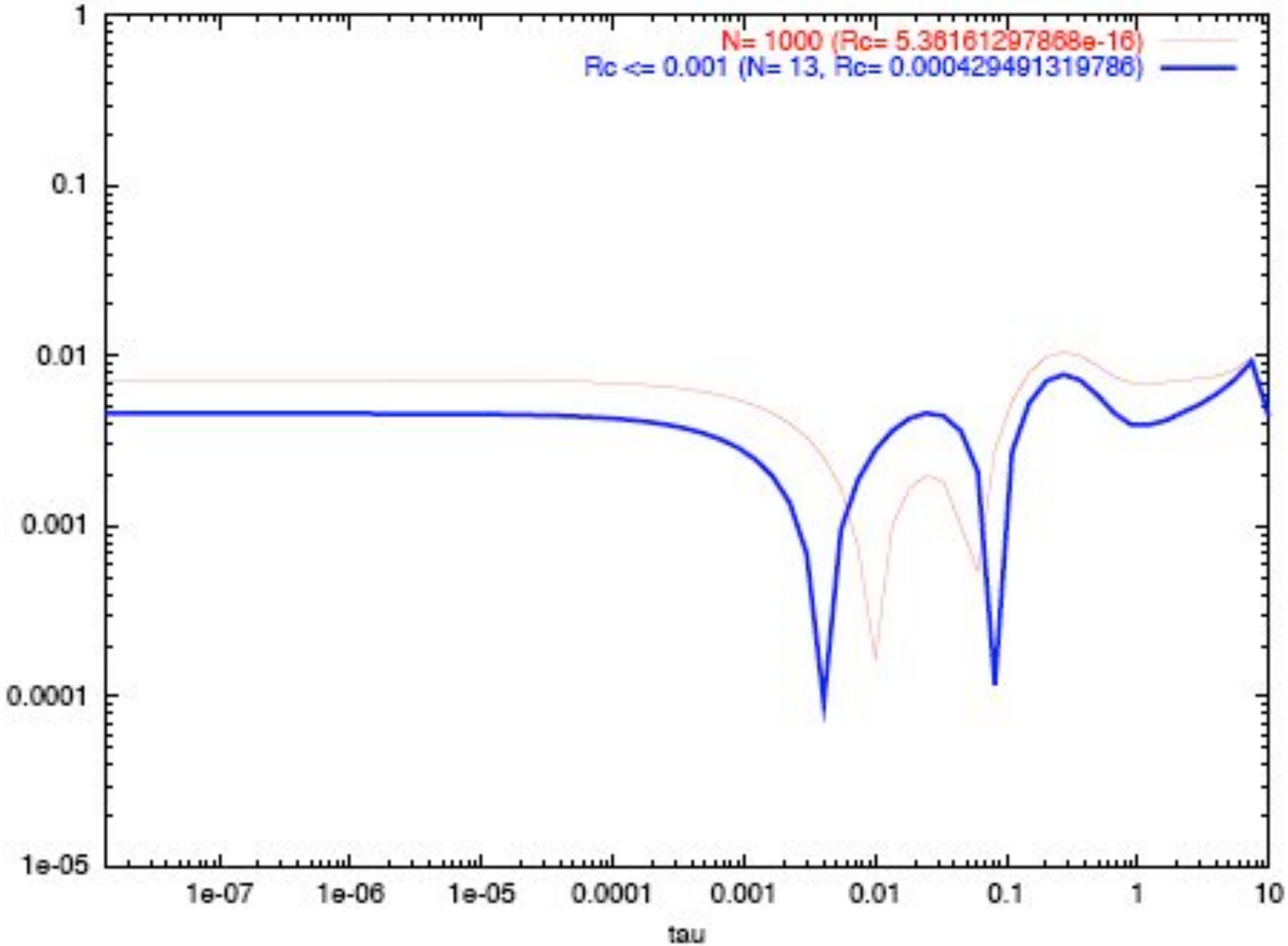
Testing ALI std parameters - B(τ) = 1 (average line)



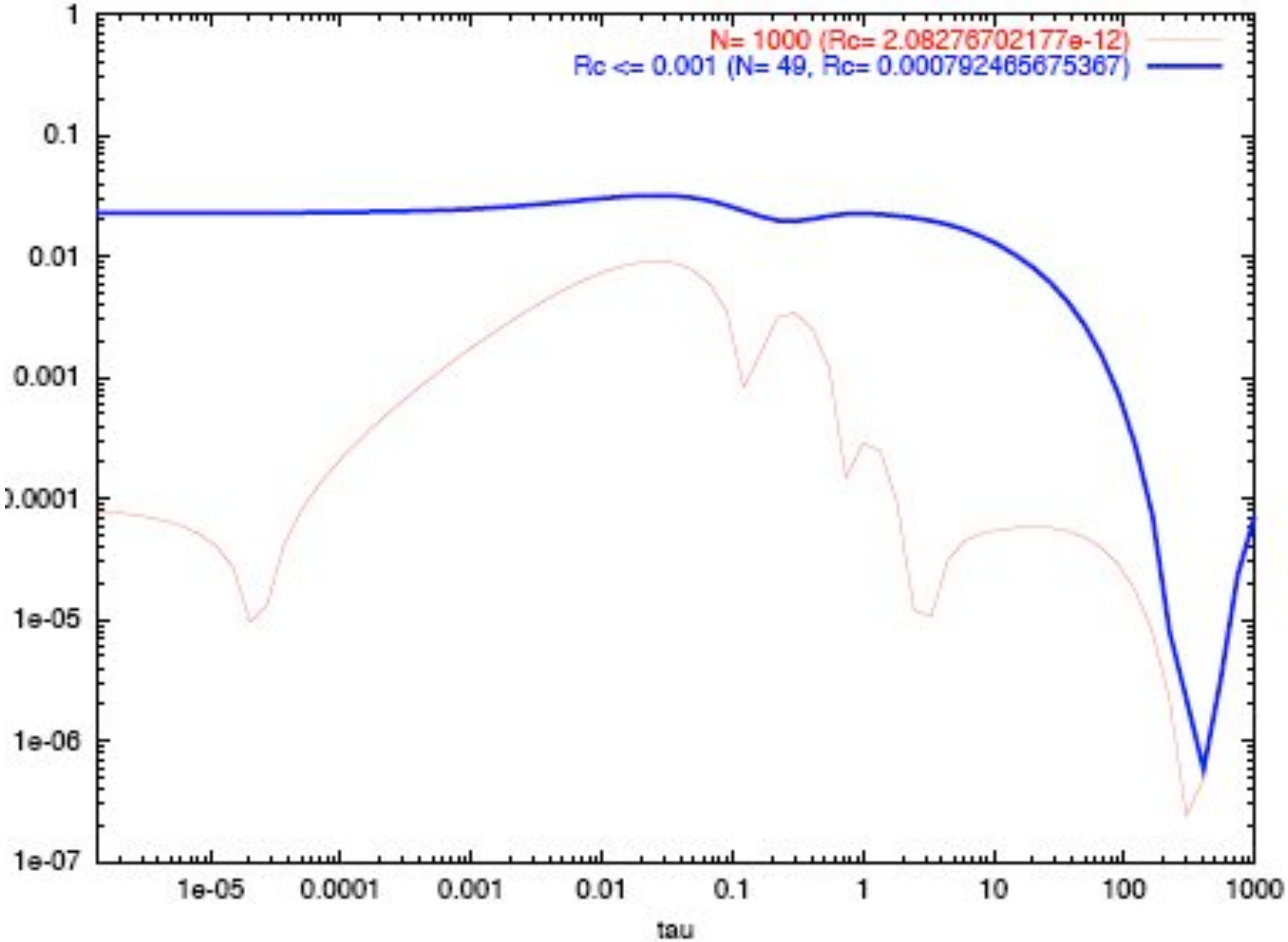
Testing ALI std parameters - B(τ) = 1 (strong line)



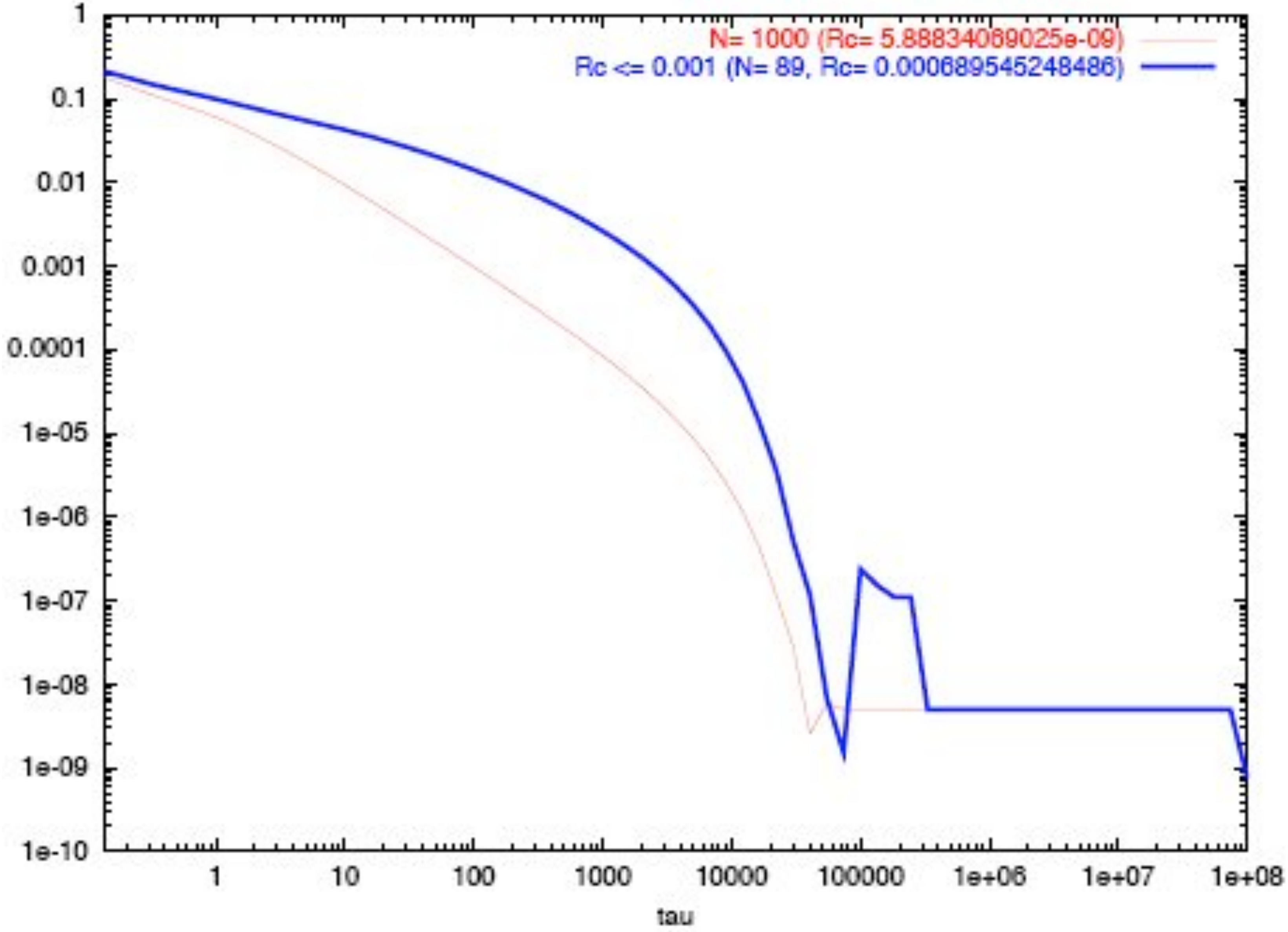
Testing ALI std parameters - $B(\tau) = \tau$ (continuum)



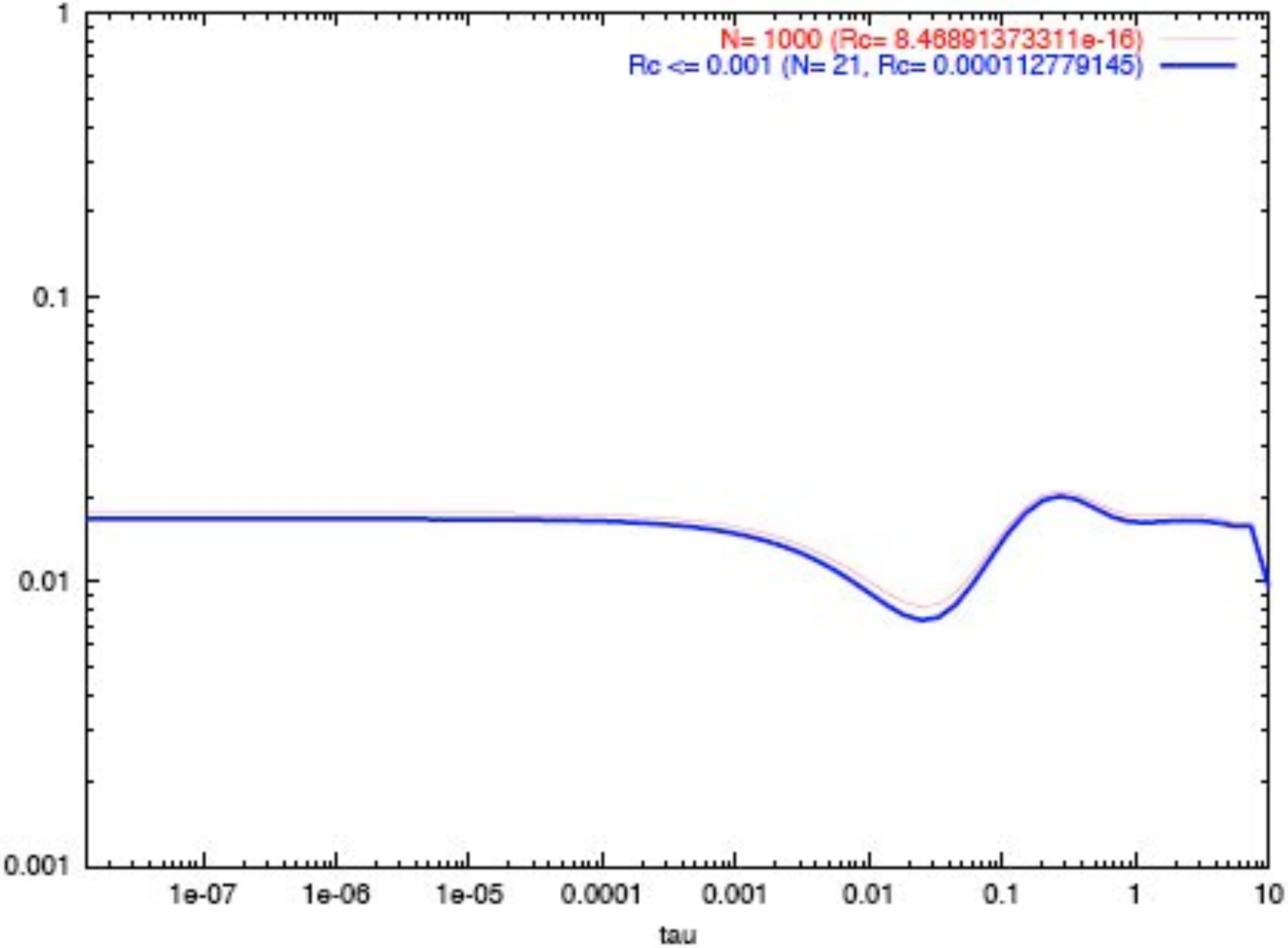
Testing ALI std parameters - $B(\tau) = \tau$ (average line)



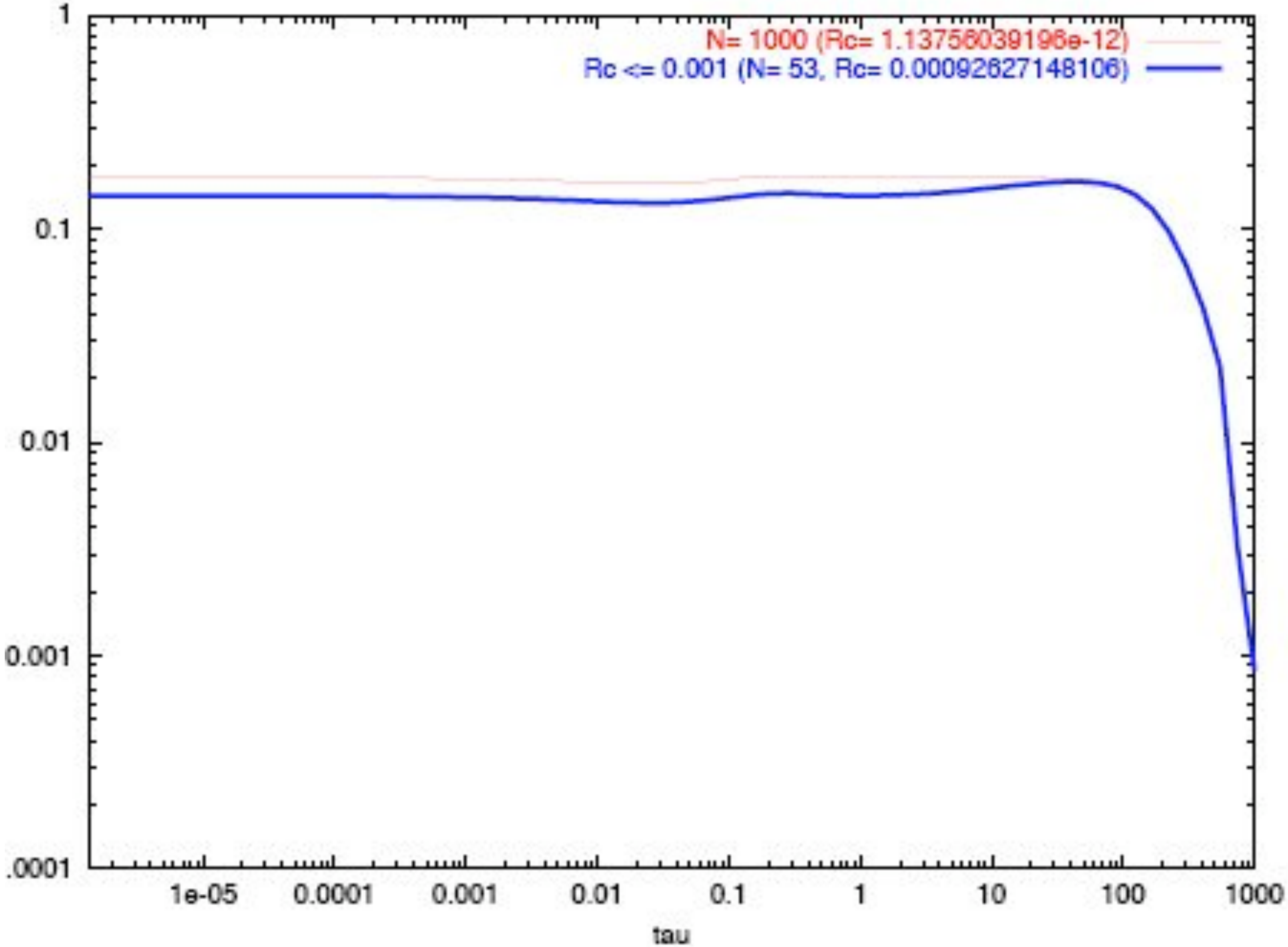
Testing ALI std parameters - B(τ) = τ (strong line)



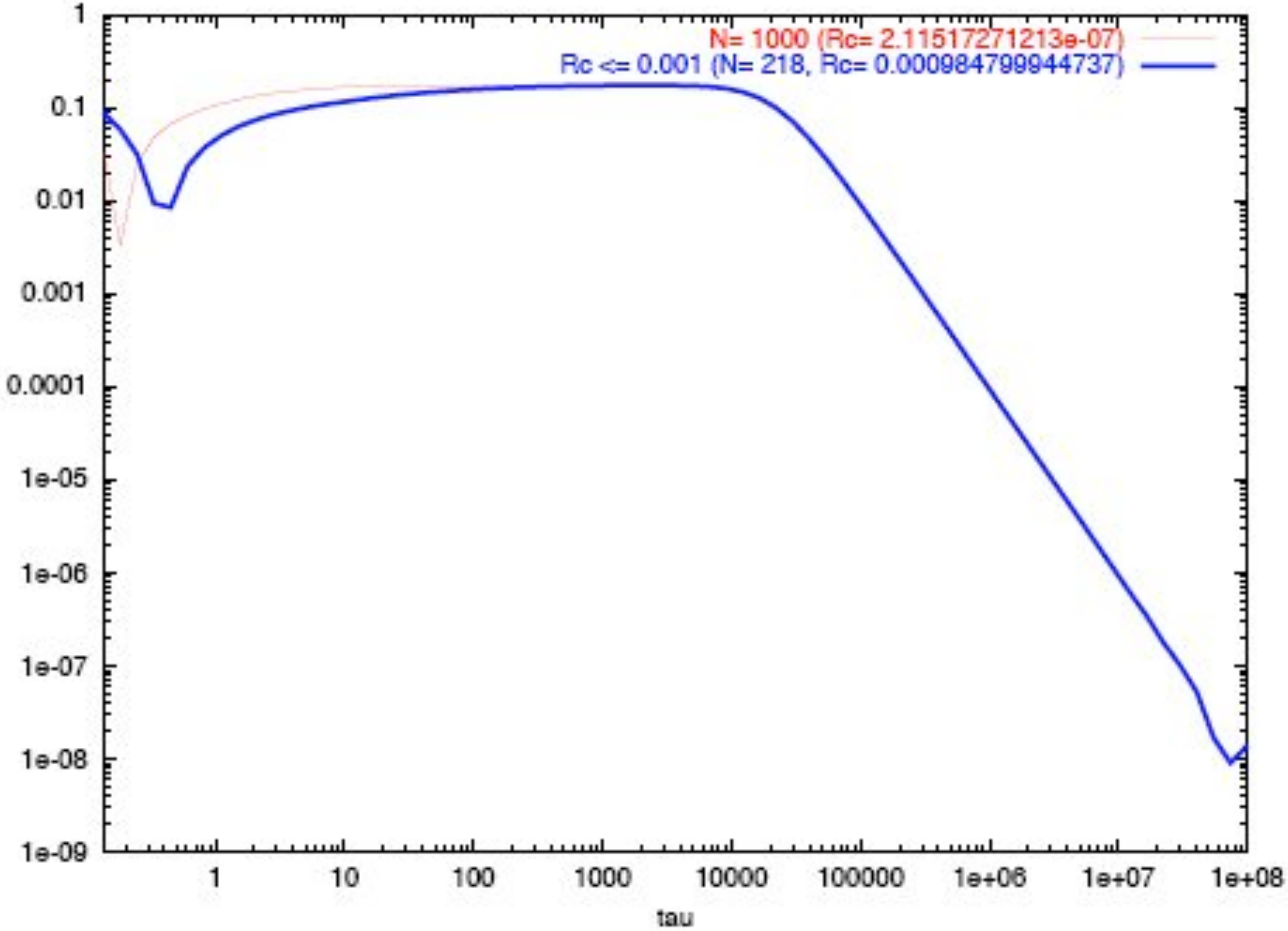
Testing ALI std parameters - $B(\tau) = \tau^5$ (continuum)



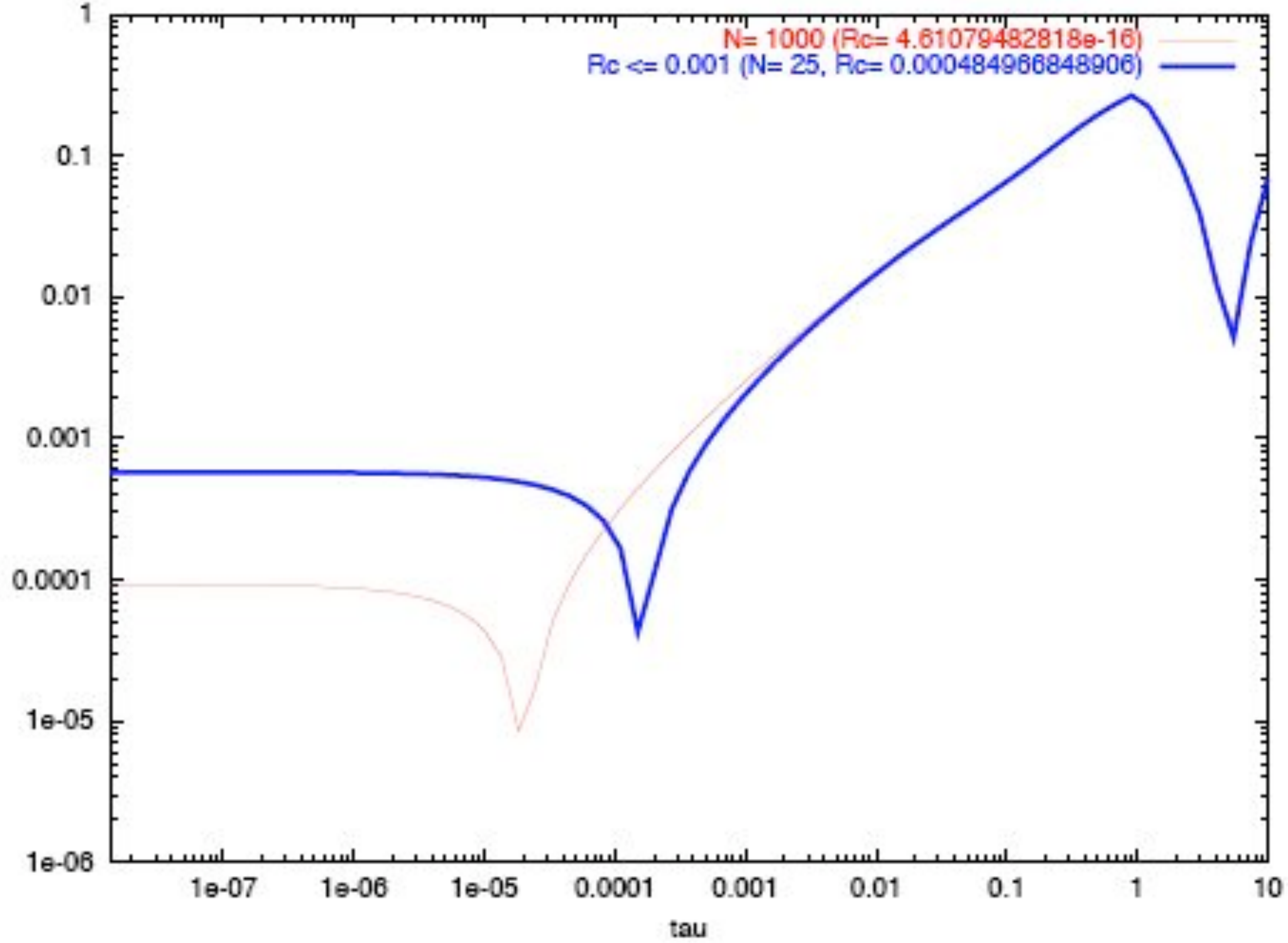
Testing ALI std parameters - $B(\tau) = \tau^5$ (average line)



Testing ALI std parameters - $B(\tau) = \tau^5$ (strong line)

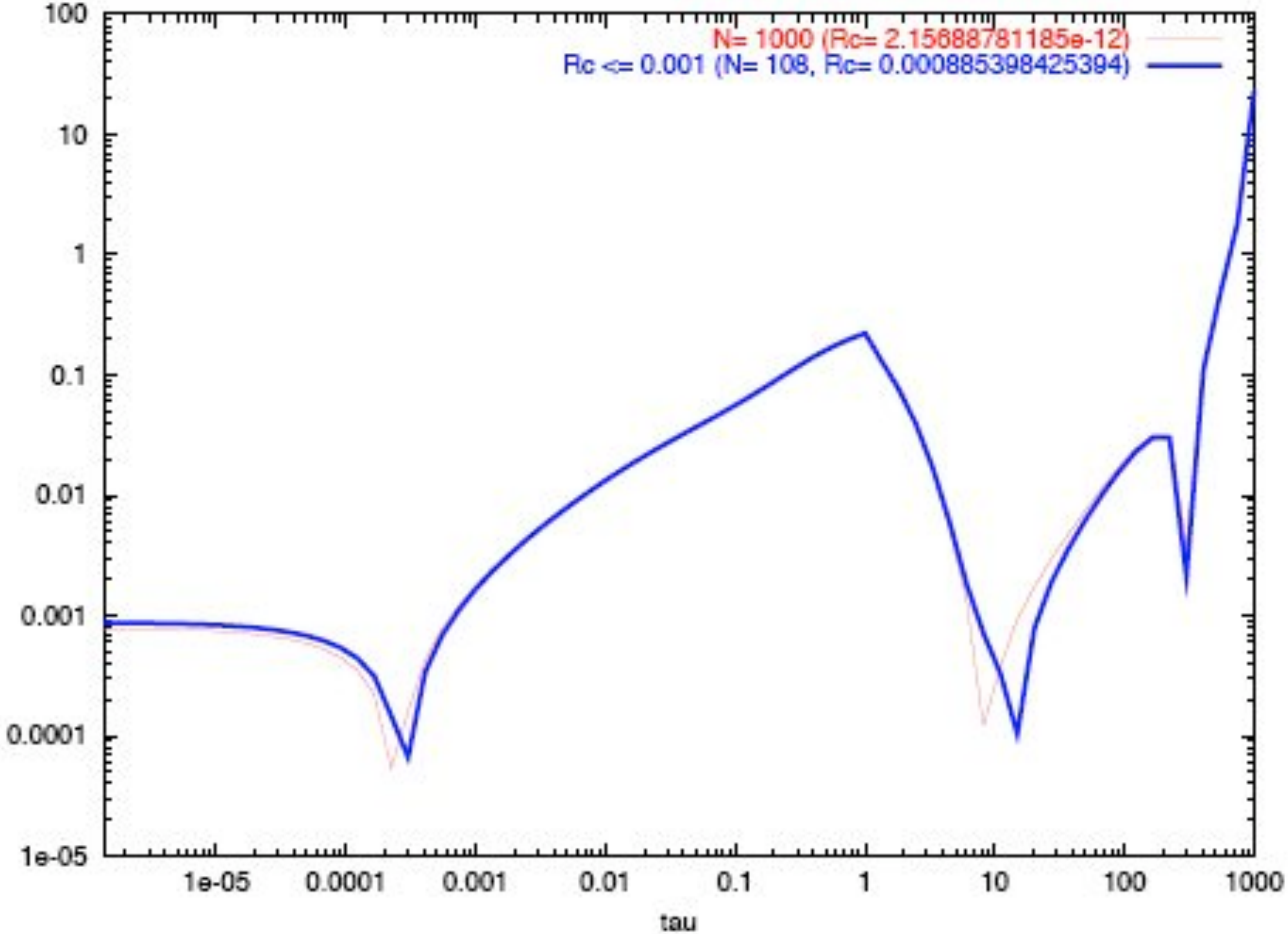


Testing ALI std parameters - $B(\tau) = \exp(-\tau)$ (continuum)

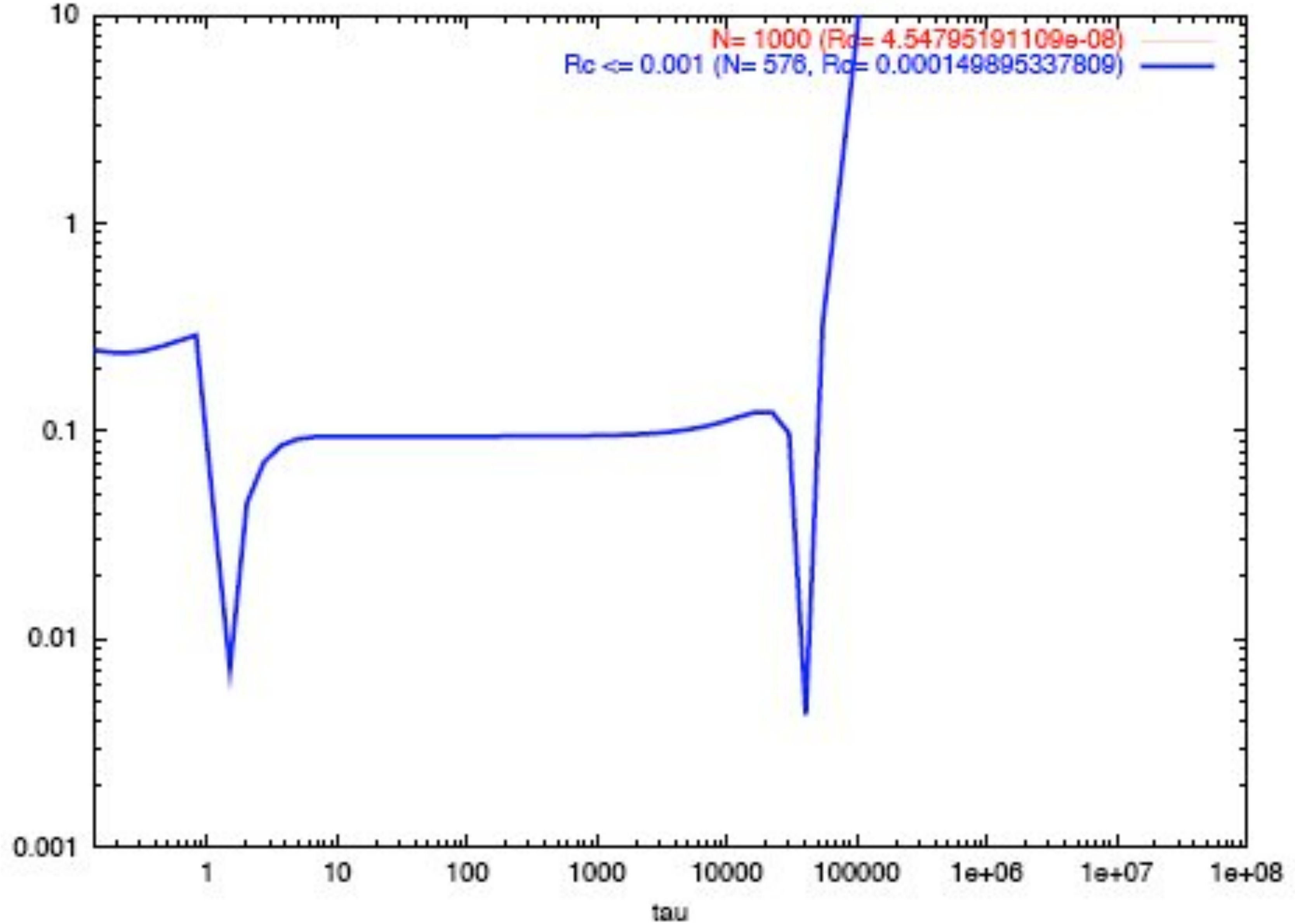


Loïc Chevallier, 30 July 2007, workshop *Non-LTE line formation for trace elements in stellar atmospheres*, Nice, France.

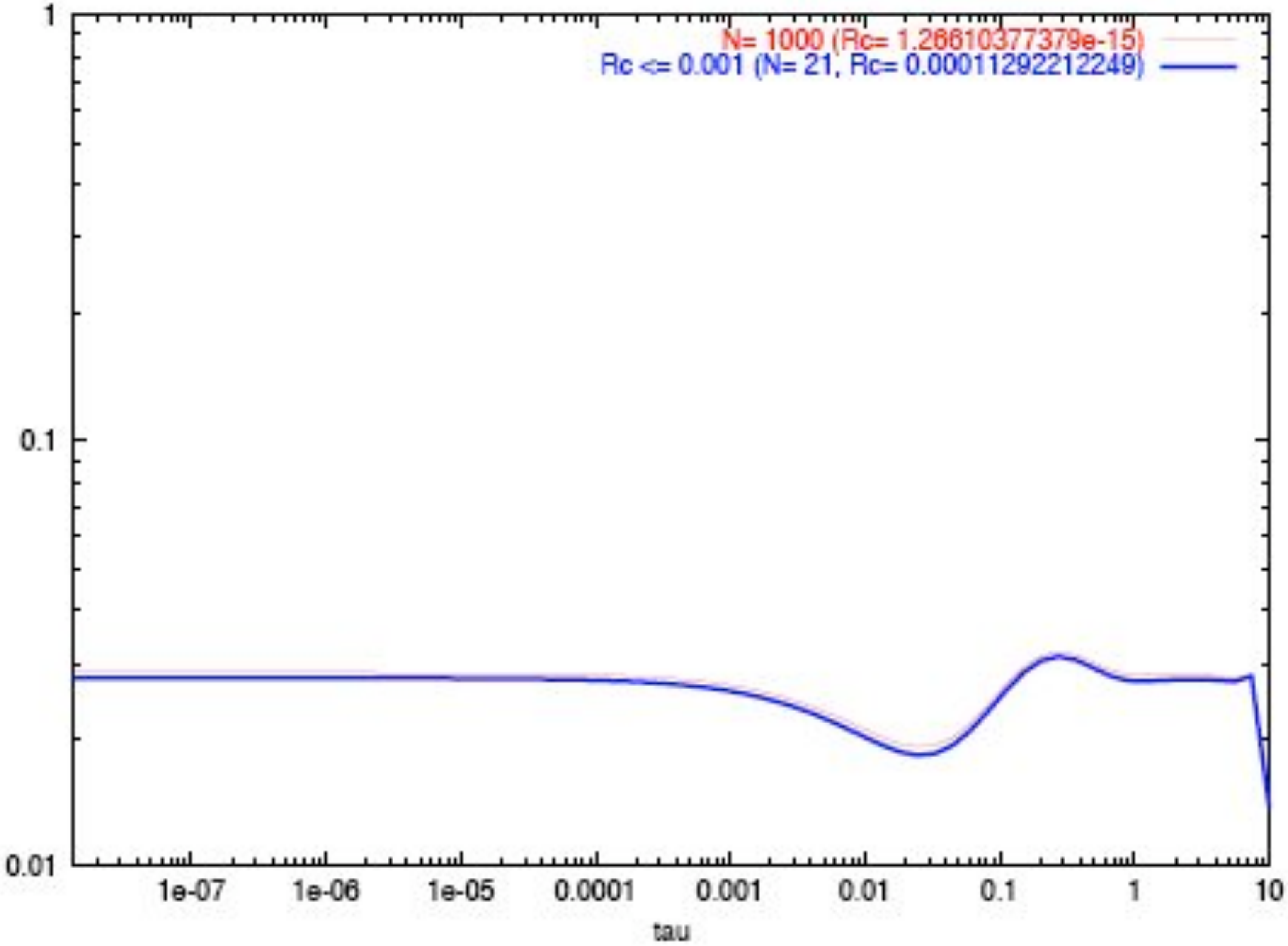
Testing ALI std parameters - B(τ) = exp(- τ) (average line)



Testing ALI std parameters - B(τ) = exp(- τ) (strong line)



Testing ALI std parameters - B(τ) = exp(τ) (continuum)



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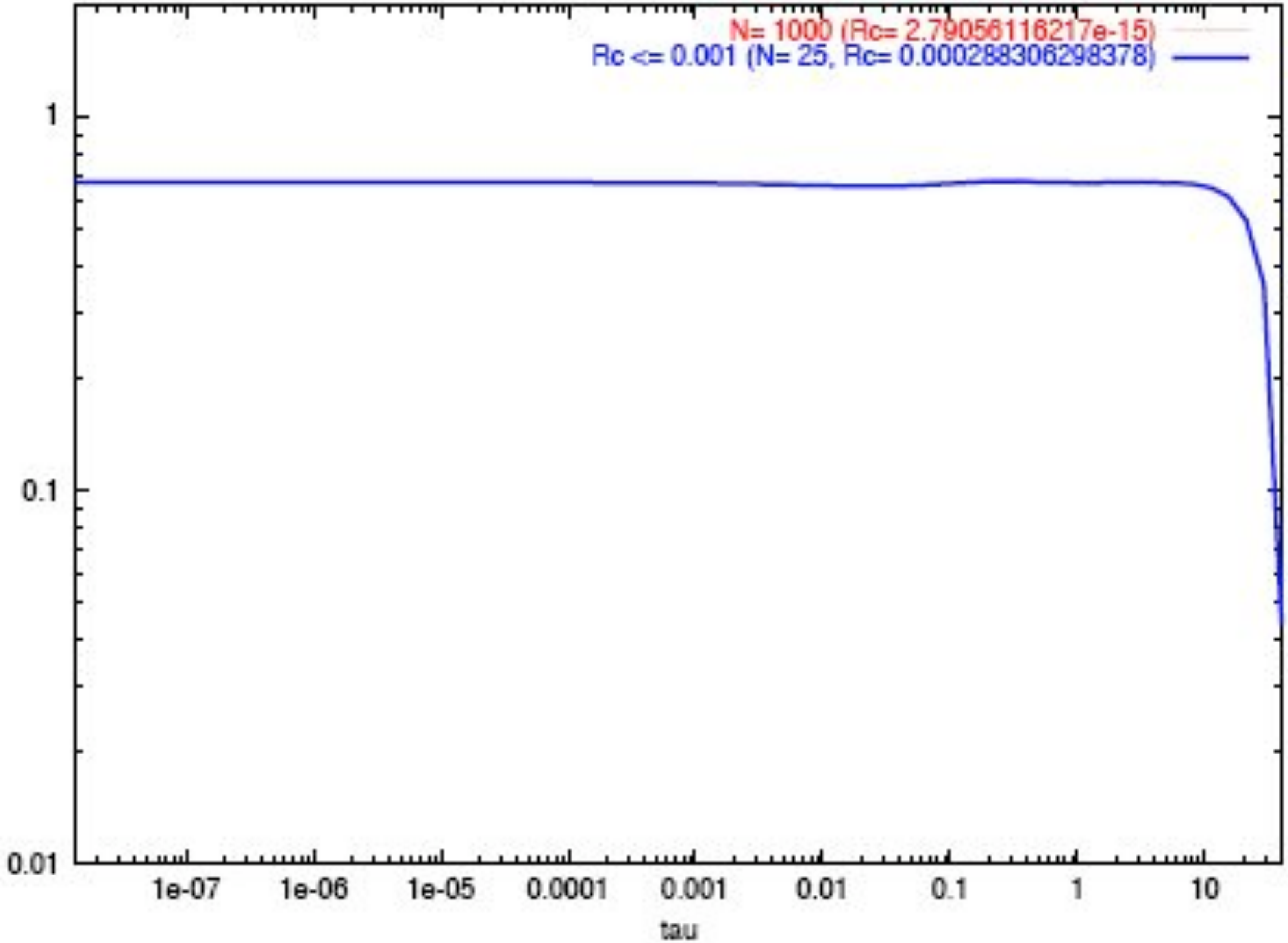

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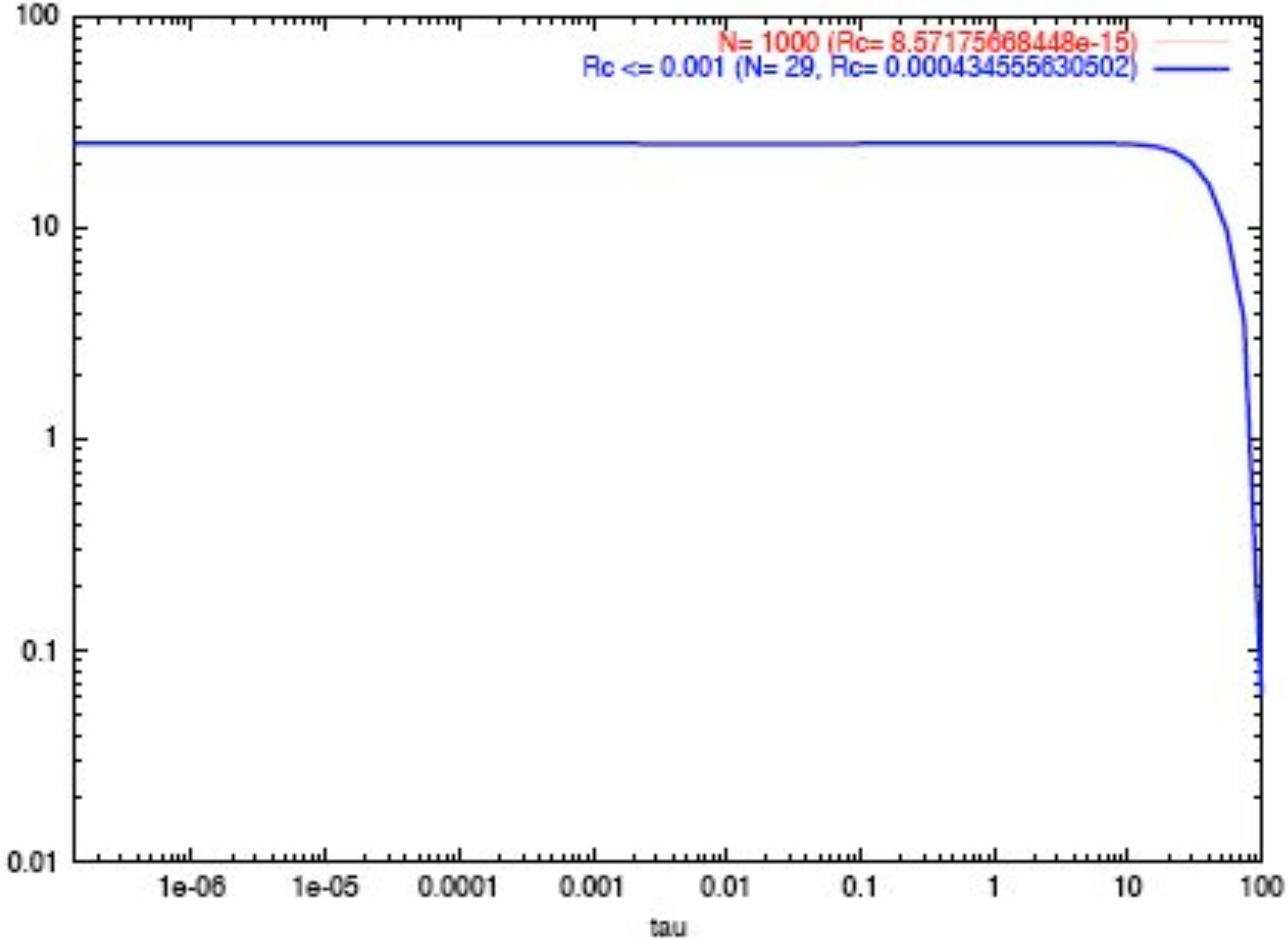

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Testing ALI std parameters - Summary

$$S_0(\tau) = (1-\varpi)B(\tau) + \frac{\varpi}{2}B(\tau^*)E_2(\tau^*-\tau)$$

<table>
<tr><td>$B(\vartheta)$</td><td>$T = 0.99$, $\vartheta^* = 10$</td><td>$\varepsilon = 1 - T = 10^{-4}$, $\vartheta^* = 1000$</td><td>$\varepsilon = 1 - T = 10^{-8}$, $\vartheta^* = 10^8$</td></tr>
<tr><td>1</td><td>0.2% - 0.7%</td><td>4%</td><td>15%</td></tr>
<tr><td>ϑ</td><td>0.5 – 0.9%</td><td>3%</td><td>20%</td></tr>
<tr><td>ϑ^5</td><td>1.5 – 2%</td><td>15 – 20%</td><td>9 – 20%</td></tr>
<tr><td rowspan="2">exp(-ϑ)</td><td colspan="3">Maximum error in the deep layers</td></tr>
<tr><td>30%</td><td>30%</td><td>30%</td></tr>
<tr><td>exp(+ϑ)</td><td>2%</td><td>$T = 0.99$, $\vartheta^* = 40$
65%</td><td>$T = 0.99$, $\vartheta^* = 100$
3000%</td></tr>
</table>

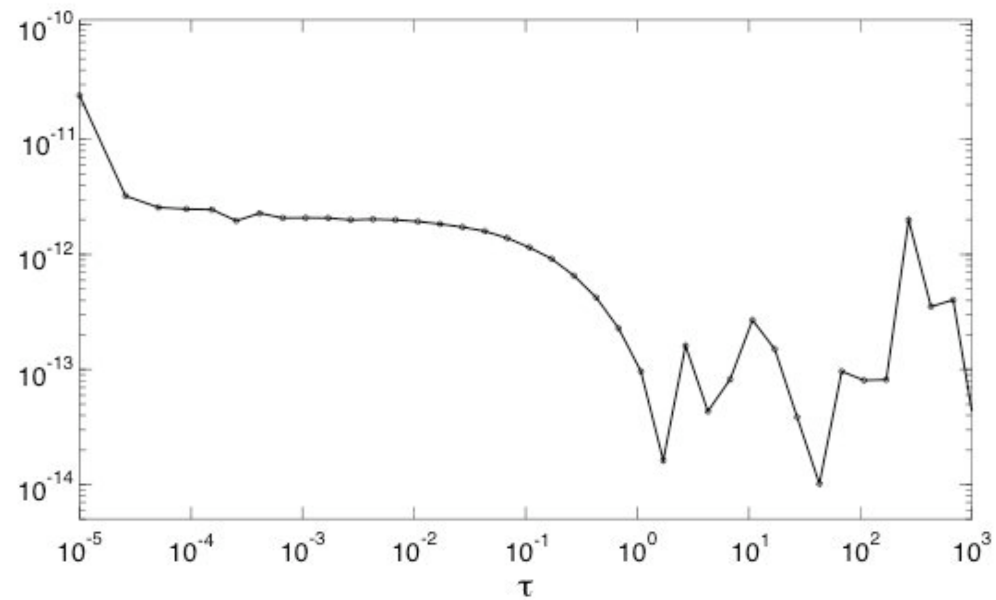
Tests ALI for some exact problems using ARTY

Chevallier et al. A&A 411, 221(2004); Chevallier (GRETA 2004)

Exact methods - ARTY

- B. Rutily (1992): exact solutions 1D (maths >16 yr, 2D, 3D possible) 12 publications TTSP, JQSRT
- Continuum and line (Milne)
- Method:
  - Finite Laplace transform,
  - complex domain,
  - integral formulation,
  - Fredholm equations regular kernel
- Code ARTY: numerical evaluation (6 yr, 300+ routines, 50 000 lines)
- NO numerical parameters (builtin)
- Applications: Atmospheres (star, planets), Benchmark, etc.

Accurate, reliable, fast



ARTY Standard relative error
Chevallier & Rutily, JQSRT (2005)

Formulation of a problem (ARTY)

Geometry and dynamics (**r**, t)

- Stationary ? YES NO
- Static ? YES NO
- Homogeneous ? YES NO
- Geometry
  - 1D
    - Plane-parallel
      - Infinite, semi-infinite, finite
    - Spherical
      - infinite, finite radius, non connexe
    - Cylindrical
      - infinite, finite radius, non connexe
  - 2D, 3D, any

Type of diffusion (**n**,ν)

- isotropical
  - conservative (albedo = 1)
  - non conservative
- anisotropical
- monochromatic
- With frequency redistribution
  - Complete redistribution
  - Partial redistribution

Classical references solutions and tests in litterature

Classical reference solutions

- $S(0) = \sqrt{\varepsilon}\ S^*(0)$, exact for isothermal semi-infinite with no illumination (Bueno et al. 1995)
- Eddington approximation semi-infinite or finite (Bueno et al. 1995)

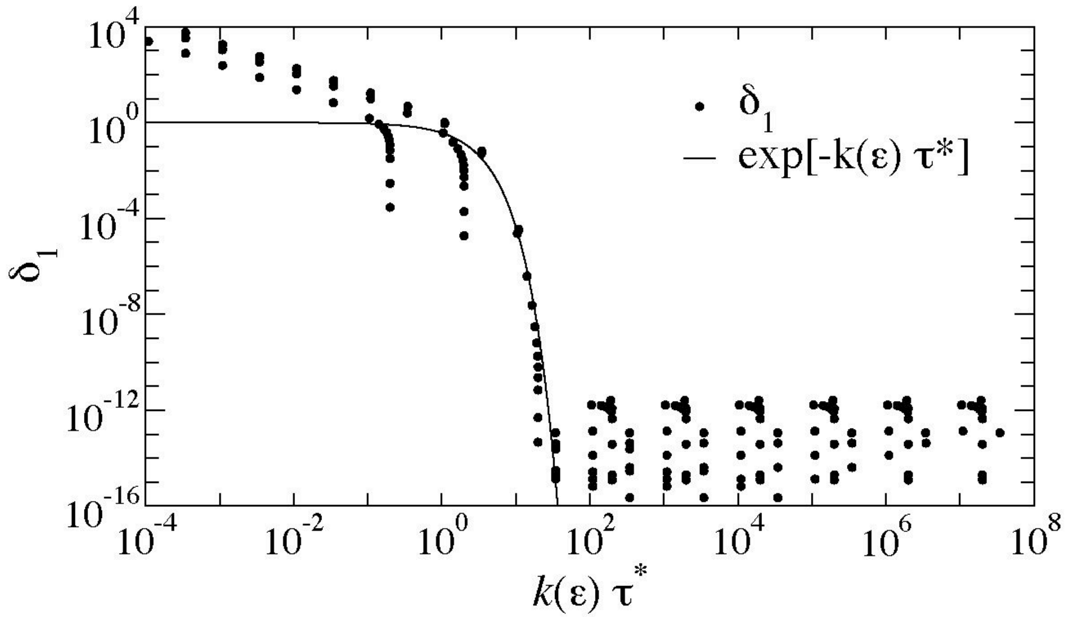
Tests in litterature (unsufficient, no exact reference solution)

- Comparison between 3 codes ε=0.5: easy (Pascucci et al. 2004)
- Comparison photoionisation codes (Pequignot et al. 2001)
- Elitzur & Asensio Ramos (2005): Escape probability, ALI
- …

Classical reference solution - √ ε-law

- point = couple (ϵ, τ^*)
- $\epsilon \in [10^{-12}, 1]$ et $\tau^* \in [0.1, 10^8]$
- $k(\epsilon) \approx \sqrt{3\epsilon}$ pour $\epsilon \to 0$ (inverse profondeur thermalisation)
- erreur $< 10^{-4}$ pour $k(\epsilon)\tau^* > 10$
- non valable continuum ($k(\epsilon)\tau^* \approx 3.3$)

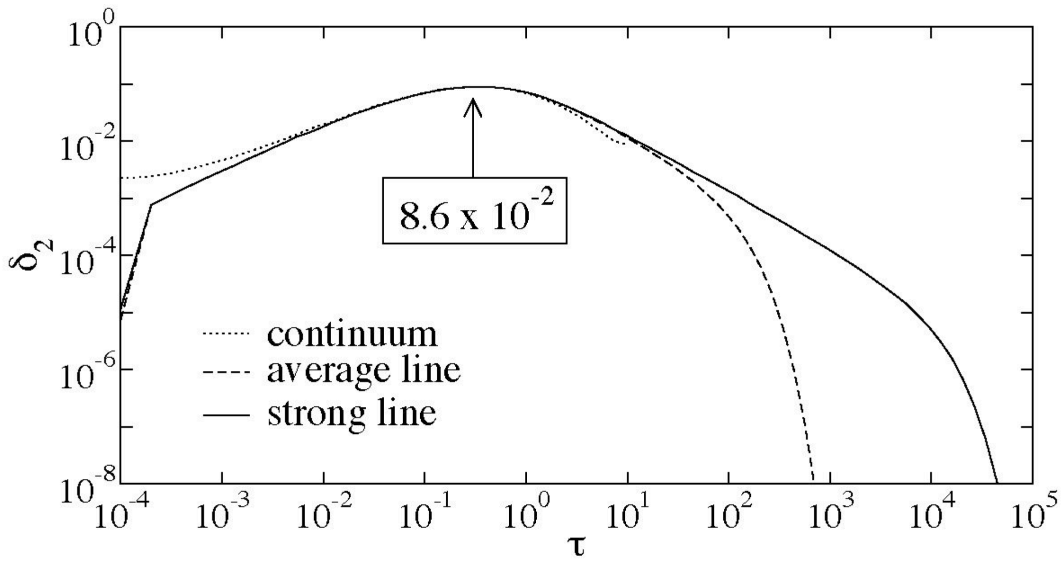
||



Classical reference solution - Eddington

- slab isotherme non éclairé
- problème intégro-différentiel $\longrightarrow$ différentiel
- erreur ALI/Eddington : 3.5×10^{-3}
- erreur Eddington : 8.6×10^{-2}
- approximation valable surface et région optiquement épaisse

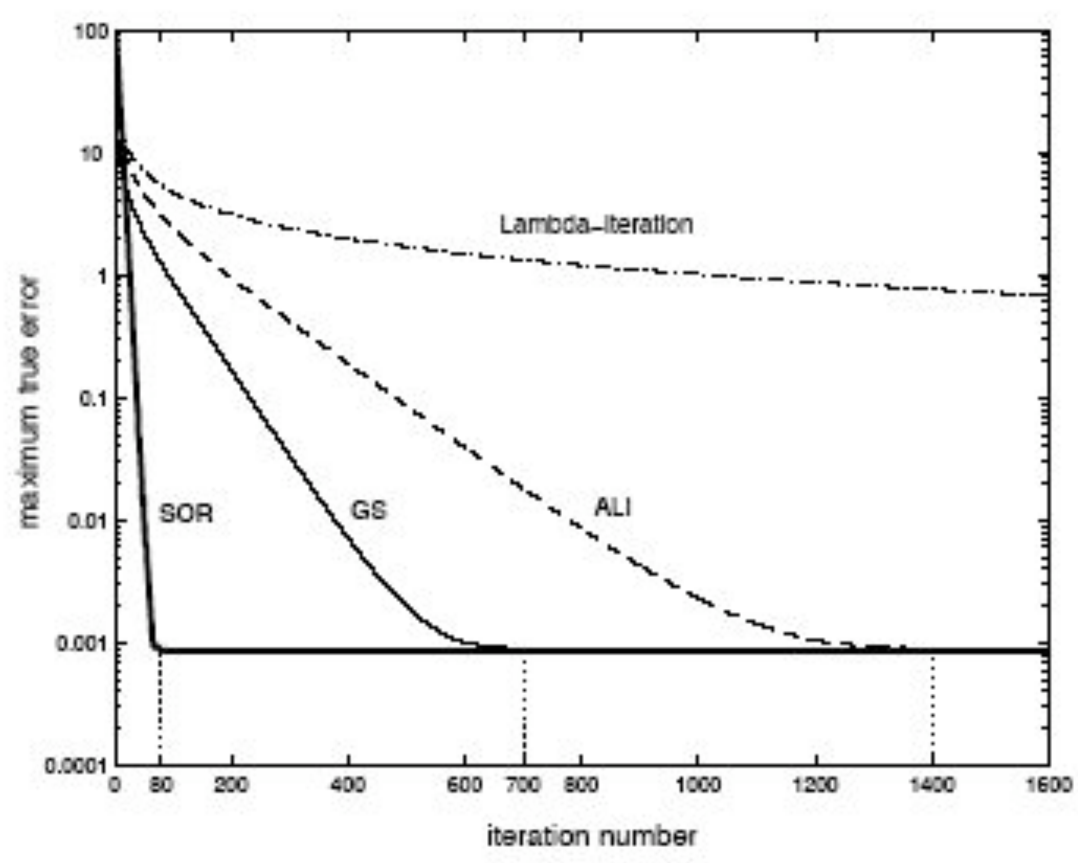
||



$$S_{\mathrm{E}}(\epsilon, \tau^*, \tau) = 1 - (1 - \epsilon) \times \frac{\exp\left(-\sqrt{3\epsilon}\,\tau\right) + \exp\left(-\sqrt{3\epsilon}\,(\tau^* - \tau)\right)}{1 + \sqrt{\epsilon} + (1 - \sqrt{\epsilon})\exp\left(-\sqrt{3\epsilon}\,\tau^*\right)}$$

ALI method (+ GS/SOR)

- 2-stream = ALI 1 angle
- ALI gives I(z,μ,ν) : 1%
- Fast robust iterative method
- Max. accuracy : z,μ-grid
- PRD, polarization, multi-D…
- Numerical parameters:
  τ, μ-grid, N (Rc), CI,
  interp. S(τ): quadratic/linear
  ⇒Needs fine tuning
- GS/SOR > x5 faster



Quang, Paletou, Chevallier (2004)
Chevallier et al., A&A (2003)

Known difficulties (solutions)

$$S(\tau) = S_0(\tau) + \varpi(\tau)\frac{1}{2}\int_0^{\tau^*} E_1(|t-\tau|)S(t)dt$$

- E_1 narrow: slow convergence (preconditioning, acceleration)
- E_1 weakly singular: $dS/d\tau(0)$ infinite (grid refinement)
- (High) gradients in S_0 (gr, linear interpolation instead parabolic)
- Optically thick spectral lines ($\tau^* >> 1$, $1-\omega << 1$) (gr)
- Iterative methods stopping criterion (multi-grid?)
- Discretization, numerical parameters (gr), roundoff errors
- Iterative methods are slow, e.g. multi-D (Krylov, parallel?)

Current status of methods (T. Lanz)

- Realistic problems: dead end, a few days to months without radiative transfer (i.e., cosmology, 3D, 7 variables)

- Idealised star (10^7 points)- cosmological simulation (10^{24} points): space (10^4-10^9), time (1-10^4), directions (10-10^4), frequencies (10-10^7)

Methods (strength, weakness)

- numerical: accurate (a few %) (less than expected), slow
  - ALI: 3ms per point per CPU (1 day - 10^{14} yr),
  - Monte-Carlo: difficulties with spectral lines (time x$10^{8\,?}$)
- approximate: fast, not accurate (for whole physical parameter space)
- Exact: fast and accurate, particular problems

TEST ALI/GS/SOR 2D
ARTY - ponctual source

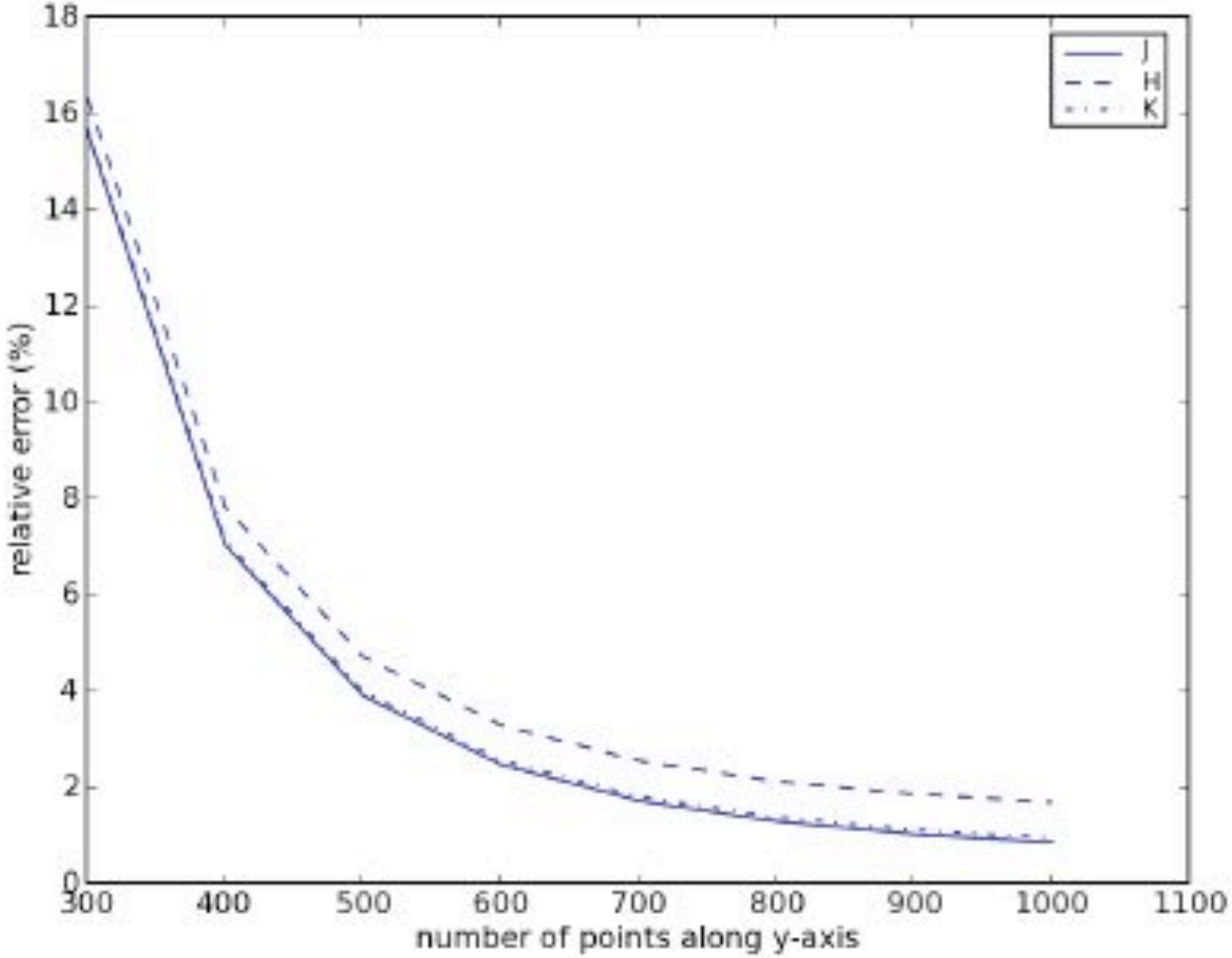


Fig. 5. Relative errors between spatial averages of the angular moments J, H and K given by the 2D-SOR 2-level iterative process and their analytical values for $\epsilon = 0.01$ vs. the number of spatial points of a square 2D grid of extension $\tau^* = 100$ in each direction.

TEST ALI/GS/SOR 2D
ARTY - ponctual source

tion time (for a Pentium-4 @ 3 GHz processor) and number of iterations for the H I multilevel benchmark mode
y_{max} = 5 000 km and z_{max} = 30 000 km together with 3 angles per octant and 8 frequencies; the temperature of t
as pressure $p_g = 1$ dyn cm^{-2}.

Points number	MALI 2D	GSM 2D	SOR 2D	MG 2D	R_c
123x123	3min9s (46)	2min19s (29)	1min17s (16)	55s (11)	1.1×10^{-2}
163x163	9min39s (79)	6min56s (48)	3min33s (24)	1min52s (13)	2.1×10^{-3}
203x203	22min47s (116)	14min36s (68)	7min34s (33)	2min50s (14)	5.7×10^{-4}
243x243	45min32s (158)	29min10s (90)	14min3s (43)	4min13s (14)	1.9×10^{-4}

Conclusion

- Solving the transfer equation is difficult but not hopeless
- Iterative methods do converge (slowly), we know some solutions for 1D
- Developping new methods, or making codes need real reference solutions (ARTY, benchmarks can be done)
- Tests available: surprises with classical numerical methods (ALI)
- Next tests: moments methods, escape probability,…

- Current work in France:
  - GRETA group (Ph. Stee) for surveys, improvements, discussion
  - ALI/GS/SOR in 1D and 2D (F. Paletou, OMP, Toulouse), CG in progress
  - Same in 3D (F. Thévenin, GAIA)
  - New 1D algorithms (CG based) with mathematicians (St Etienne, France; Moscow)

- Radiative transfer developments (independent of a given problem) should be a research thema for astrophysicists