GYRE: Yet another oscillation code, why we need it and how it works

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What might one want from a new code?

- Improved flexibility to handle new problems
  - oscillations with differential rotation & magnetic fields
  - dynamic tides in binary stars
- Greater accuracy and robustness
  - "hands-off" asteroseismic analyses
  - integrated oscillation & stellar evolution simulations
- Higher performance
  - Take advantage of multiple cores / nodes

GYRE: A new oscillation code suite

- Programmatic motivation: developed as part of "*Wave transport of angular momentum: a new spin on massive-star evolution*" (NSF grant #AST 0908688)

- Personal motivations:
    - why does the BOOJUM code (Townsend 2005) work in cases x and y, but not in case z?
    - I enjoy programming!

Statement of the problem

- Stellar oscillation is a linear two-point boundary-value problem (BVP):

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}x} = \mathsf{A}(x)\,\mathbf{y}$$

$$\mathsf{B}_a\,\mathbf{y}_a \equiv \mathsf{B}_a\,\mathbf{y}(x_a) = 0$$

$$\mathsf{B}_b\,\mathbf{y}_b \equiv \mathsf{B}_b\,\mathbf{y}(x_b) = 0$$

- The problem specifics are defined by the Jacobian matrix A and the boundary conditions B

Alternative approaches to solving BVPs

Shooting

Smeyers (1966, 1967)

Relaxation

Castor (1970)

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<u>At a fundamental level, both approaches are the same!</u>

Relaxation

- Replace the differential equations by finite differences on a discrete grid $x = x^k$ ($k = 1,\ldots,N$):

$$\frac{\mathbf{y}^{k+1} - \mathbf{y}^k}{x^{k+1} - x^k} = \mathsf{A}\left(\frac{x^{k+1} + x^k}{2}\right)\frac{\mathbf{y}^{k+1} + \mathbf{y}^k}{2}$$

- Combine the difference equations with the boundary conditions to form a large, sparse linear system for $\mathbf{y}^k$

Shooting via superposition

- Use initial-value problem (IVP) integrator to solve

$$\frac{\mathrm{d}\mathsf{Y}}{\mathrm{d}x} = \mathsf{A}(x)\mathsf{Y}, \quad \mathsf{Y}(x_a) = \mathsf{I}$$

- The fundamental solution Y relates $\mathbf{y}^b$ back to $\mathbf{y}^a$:

$$\mathbf{y}^b = \mathsf{Y}(x^b)\,\mathbf{y}^a$$

- The BVP becomes a linear system for $\mathbf{y}^a$:

$$\mathsf{B}^a\,\mathbf{y}^a = 0$$

$$\mathsf{B}^b\mathsf{Y}(x^b)\,\mathbf{y}^a = 0$$

Multiple shooting: the best of both worlds

- Apply shooting across multiple intervals of a discrete grid $x = x^k$ $(k = 1,\ldots,N)$:

$$\mathbf{y}^{k+1} = \mathsf{Y}(x^{k+1}; x^k)\,\mathbf{y}^k$$

- Combine with the boundary conditions to form large, sparse linear system for $\mathbf{y}^k$

- Stability is improved vs. single/double shooting

- Depending on how we evaluate $\mathsf{Y}^{k+1,k} = \mathsf{Y}(x^{k+1};x^k)$, accuracy is improved vs. relaxation

- Multiple shooting is easy to parallelize

Calculating the fundamental solution matrices

- Simple approach following Gabriel & Noels (1976): assume the Jacobian matrix $\mathsf{A}(x)$ is constant in each interval $x^k \leq x \leq x^{k+1}$

- The fundamental solution matrix is then a matrix exponential:

$$\mathsf{Y}^{k+1;k} = \exp\left\{[x^{k+1} - x^k]\mathsf{A}\right\}$$

- This approach has *arbitrarily high resolution* of eigenfunction oscillations

- However, it is only second-order accurate

Higher-order approaches using the Magnus method

- Magnus (1954): solutions to the IVP

$$\frac{\mathrm{d}\mathsf{Y}}{\mathrm{d}x} = \mathsf{A}(x)\mathsf{Y}, \quad \mathsf{Y}(x_a) = \mathsf{I}$$

can be written as

$$\mathsf{Y} = \exp\{\mathsf{M}(x)\}$$

- The Magnus matrix M can be expanded as an infinite series, with leading terms

$$\mathsf{M}(x) = \int_{x_a}^{x} \mathsf{A}(x_1)\,\mathrm{d}x_1 - \frac{1}{2}\int_{x_a}^{x}\left[\int_{x_a}^{x_1} \mathsf{A}(x_2)\,\mathrm{d}x_2, \mathsf{A}(x_1)\right]\mathrm{d}x_1 + \ldots$$

Magnus methods in GYRE

- Integrals in the Magnus expansion are evaluated using Gauss-Legendre quadrature
- Matrix exponentials are evaluated via a spectral decomposition of M:

$$\exp \mathsf{M} = \mathsf{U}(\exp \Lambda)\mathsf{U}^{-1}$$

- Three choices in GYRE:
  - MAGNUS_GL2 – 2^{nd} order (Gabriel & Noels approach)
  - MAGNUS_GL4 – 4^{th} order
  - MAGNUS_GL6 – 6^{th} order

Stellar oscillation is an eigenproblem

- The oscillation equations appear to be over-determined:
  - 4 differential equations (adiabatic case)
  - 4 boundary conditions
  - 1 arbitrary normalization condition
- The BVP can only be solved at discrete values of the oscillation frequency ω appearing in the Jacobian matrix
- These discrete values are the *eigenfrequencies*; the corresponding solutions are the *eigenfunctions*

Castor's method

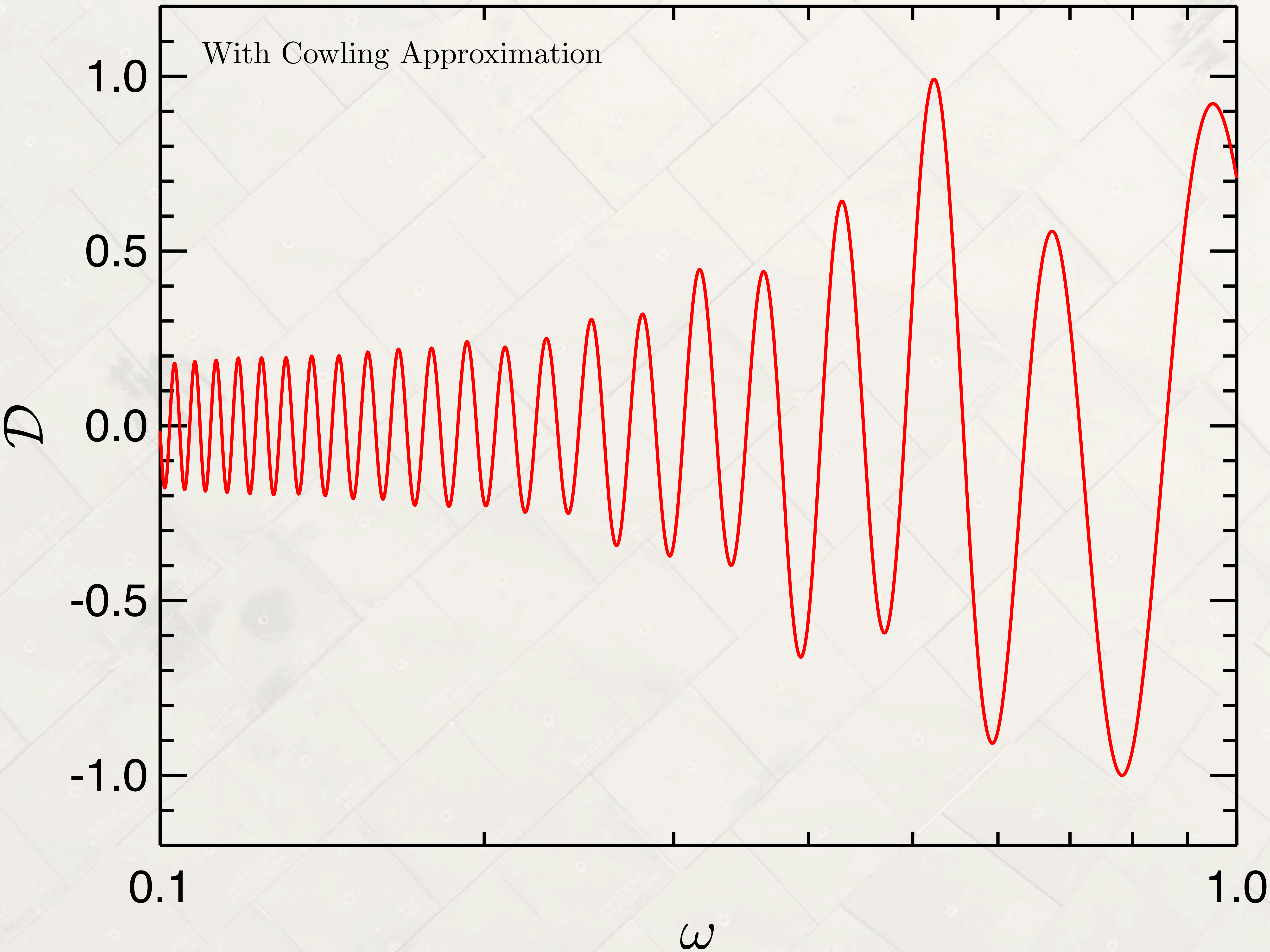
- Replace one of the boundary conditions with the normalization condition

- The BVP can then be solved for any value of the frequency ω

- Use the neglected boundary condition to define a discriminant function $D(\omega)$, such that D is zero when the boundary condition is satisfied

- The roots of $D(\omega)$ then correspond to the stellar eigenfrequencies

Ill-behaved discriminants: The downfall of Castor's method



This problem can affect *any* code which involves a single-point determinant (e.g., GraCo; PULSE; ADIPLS; NOSC)

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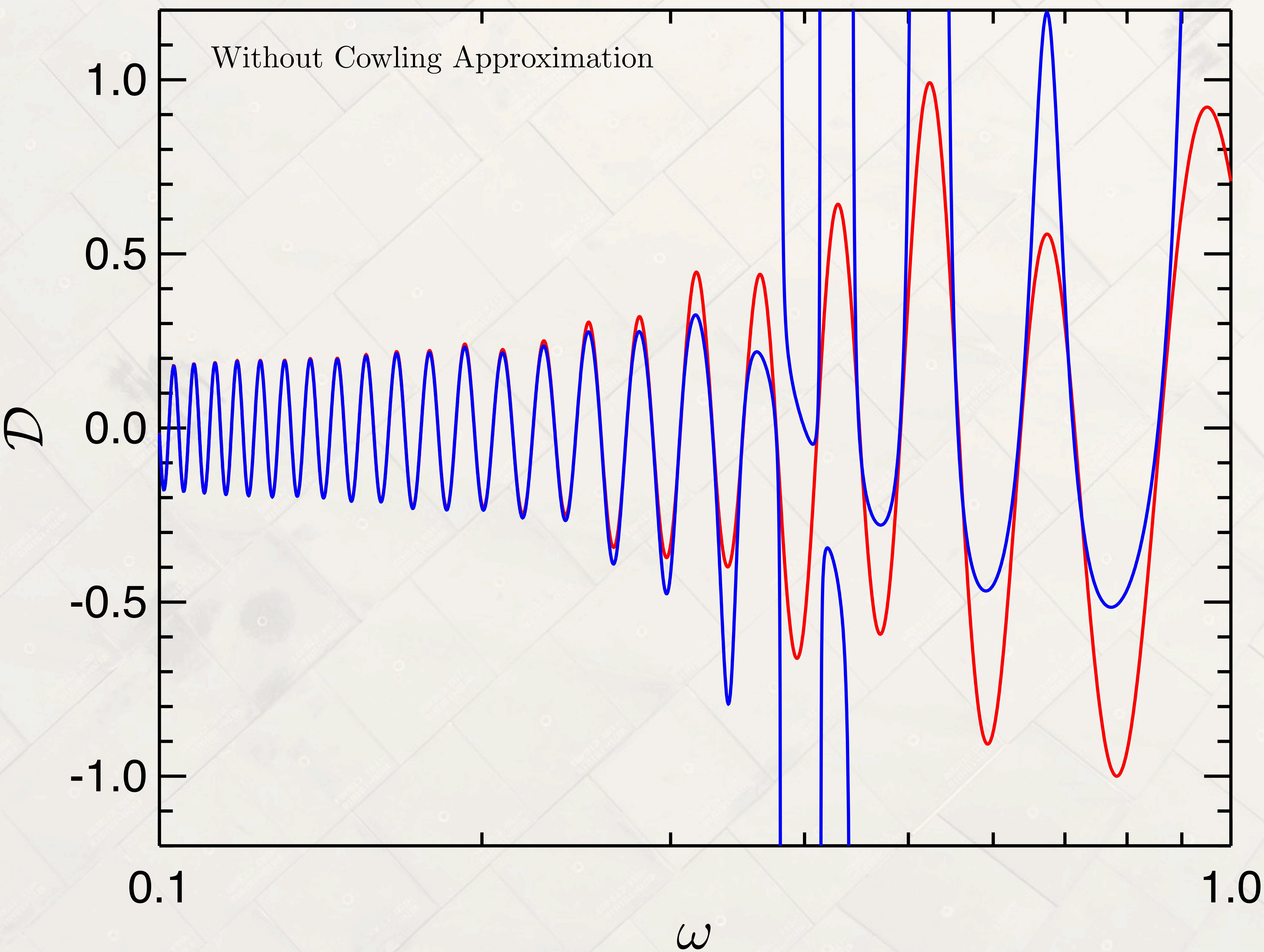


This problem can affect *any* code which involves a single-point determinant (e.g., GraCo; PULSE; ADIPLS; NOSC)

Recognizing the problem

- The equations plus boundary conditions can be written as a linear, homogeneous system:

$$\mathsf{S}\,\mathbf{u} = 0$$

$$\mathsf{S} = \begin{pmatrix} \mathsf{B}^a & 0 & 0 & \cdots & 0 & 0 \\ -\mathsf{Y}^{2;1} & \mathsf{I} & 0 & \cdots & 0 & 0 \\ 0 & -\mathsf{Y}^{3;2} & \mathsf{I} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\mathsf{Y}^{N;N-1} & \mathsf{I} \\ 0 & 0 & 0 & \cdots & 0 & \mathsf{B}^b \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} \mathbf{y}^1 \\ \mathbf{y}^2 \\ \vdots \\ \mathbf{y}^N \end{pmatrix}$$

Solution of linear, homogeneous systems

- *Any* system of linear, homogeneous equations admits non-trivial solutions ($\mathbf{u} \neq \mathbf{0}$) when the determinant of the matrix S vanishes

- Hence, the determinant can be adopted as the discriminant function:

$$D(\omega) = \det \mathsf{S}$$

- The determinant is a polynomial in the components of S; if these components are well behaved, then so is D

Evaluating the determinant in GYRE

- LU decompose the system matrix

$$\mathsf{S} = \mathsf{L}\,\mathsf{U}$$

- Form the determinant as the diagonal product

$$\det \mathsf{S} = \prod_i \mathsf{U}_{i,i}$$

- Wright (1994, *Numer. Math.* **67**, 521) gives a parallel algorithm for LU decomposition, which performs well on shared-memory systems

Dealing with determinant overflow

"For a matrix of any substantial size, it is quite likely that the determinant will overflow or underflow your computer's floating point dynamic range"

Numerical Recipes in Fortran, 2nd ed., "Determinant of a Matrix"

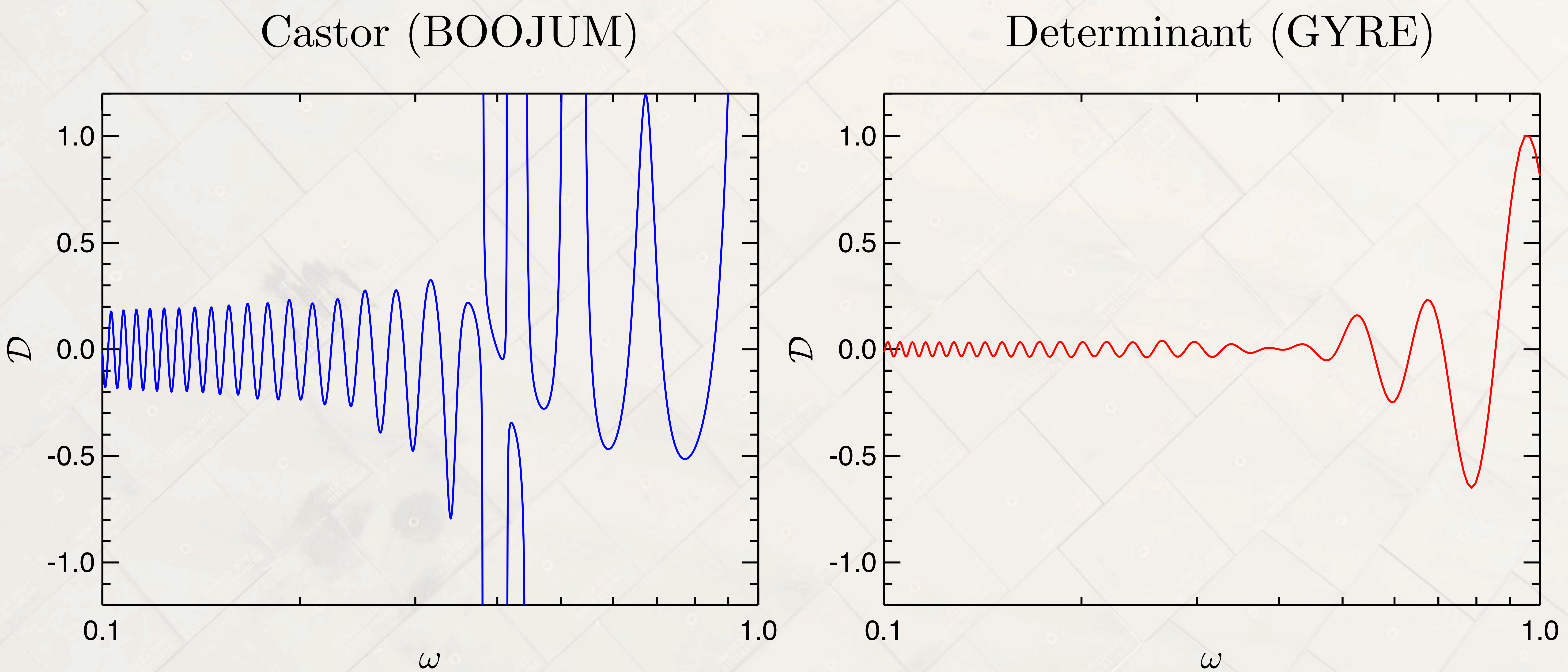
Solution: use extended-precision arithmetic

$$x = f \times 2^e \qquad \begin{array}{ll} f \in \mathbb{R}, & 0.25 < f \leq 0.5 \\ e \in \mathbb{Z}, & |e| \leq 2147483647 \end{array}$$

Summarizing the GYRE approach

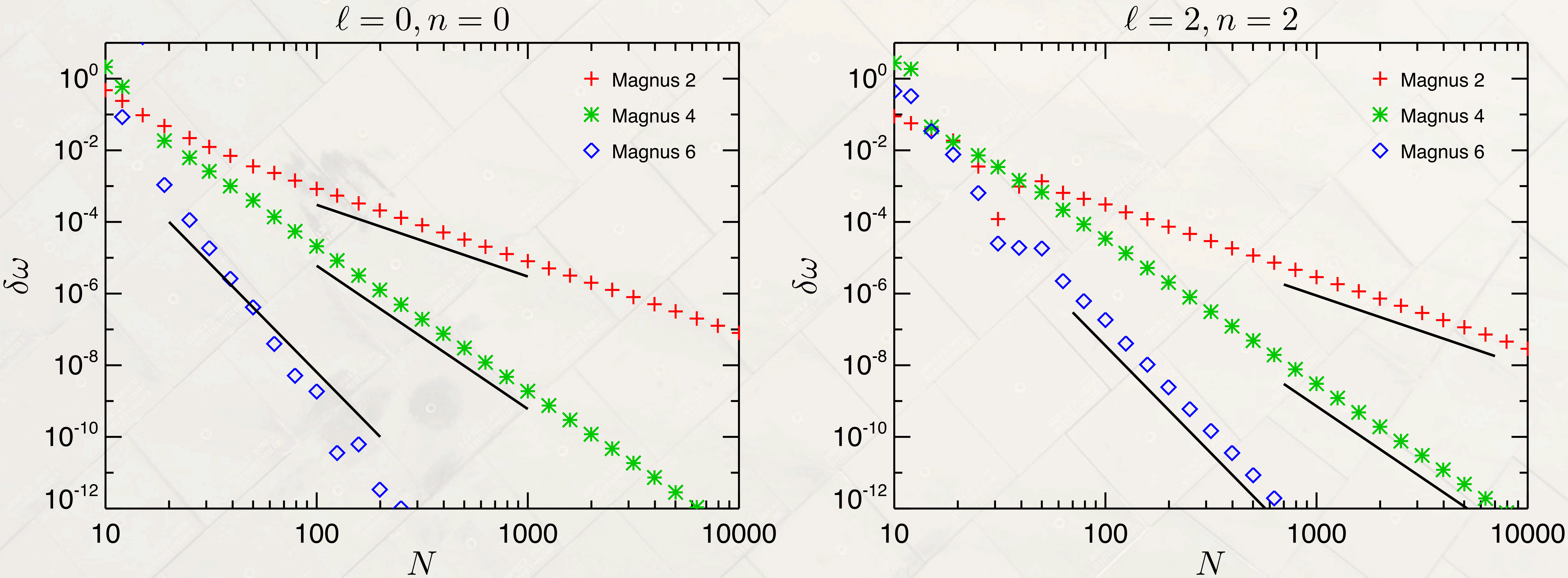
- GYRE uses a *Magnus multiple shooting* (MMS) scheme for BVPs
- Multiple shooting is used for robustness & performance
- Magnus methods are used for accuracy
- A determinant-based discriminant avoids the problems of Castor's method
- The code is parallelized with both Open MP and MPI

Old vs. new discriminants



<u>Both discriminants have the same roots; but the determinant-based discriminant is well behaved</u>

Testing convergence with the $n = 0$ polytrope



For each Magnus method, the error in the eigenfrequency has the expected scaling

Comparison against ESTA results

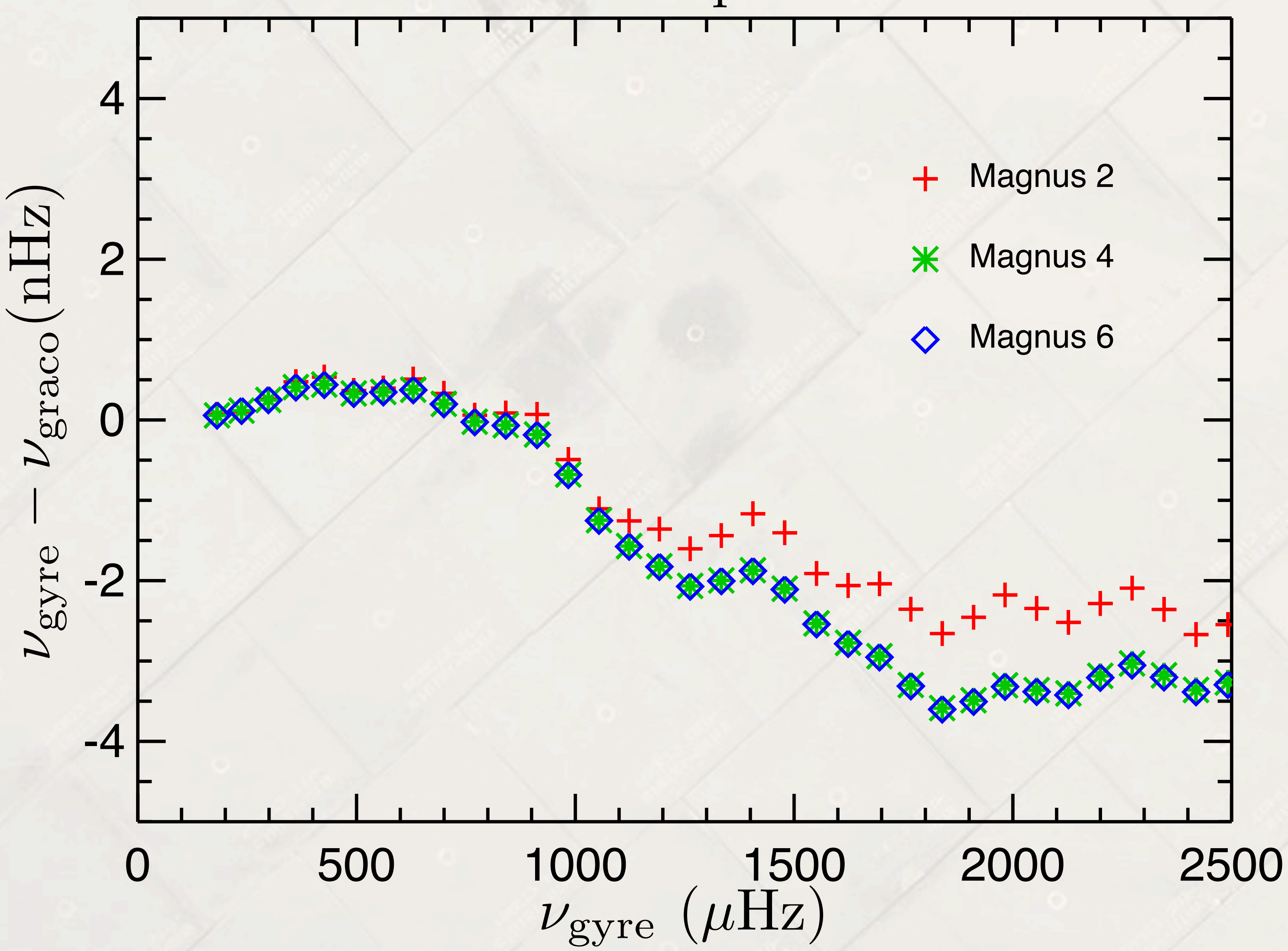
Astrophys Space Sci (2008) 316: 231–249
DOI 10.1007/s10509-007-9717-z

ORIGINAL ARTICLE

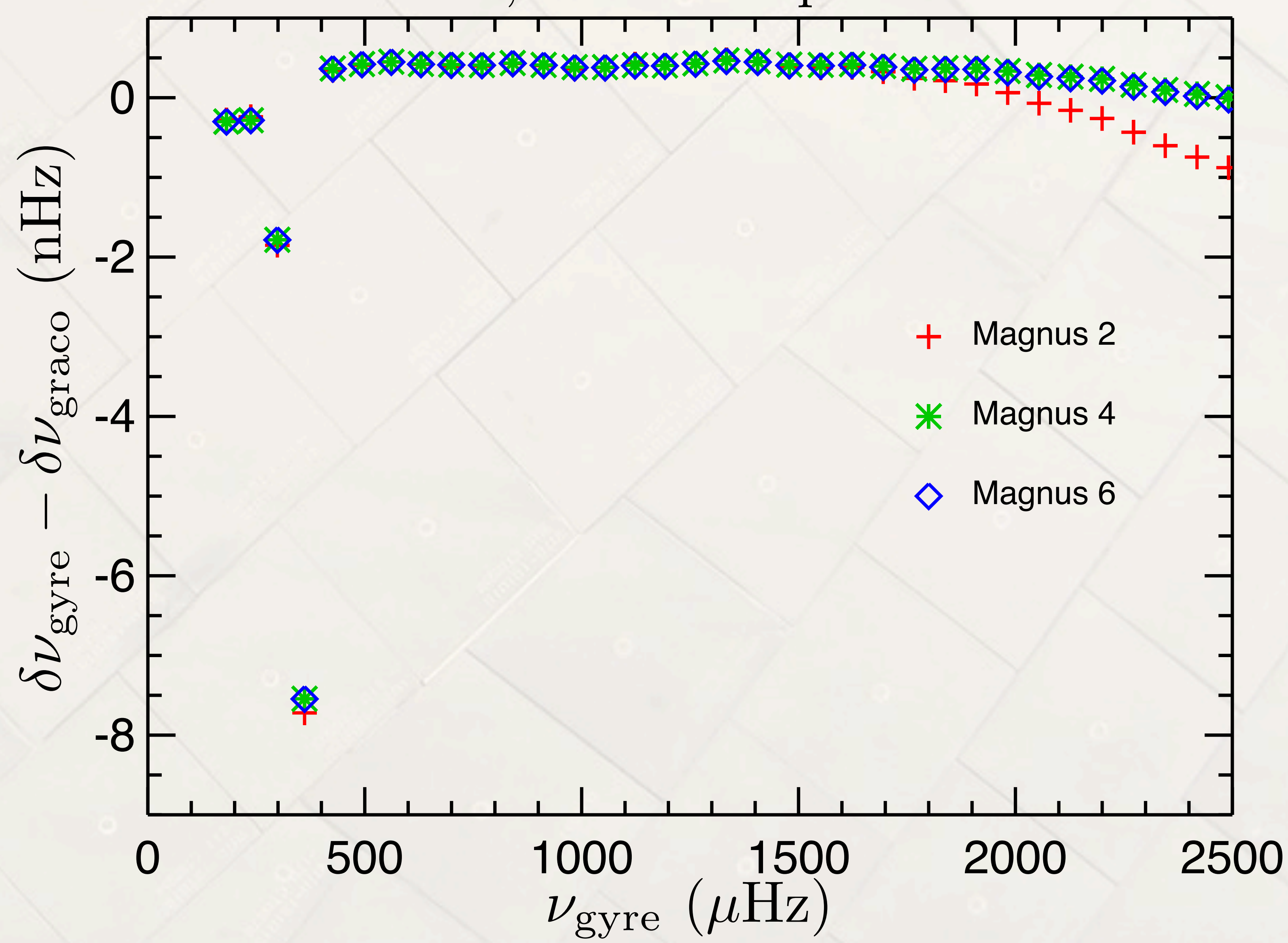
Inter-comparison of the g-, f- and p-modes calculated using different oscillation codes for a given stellar model

A. Moya · J. Christensen-Dalsgaard · S. Charpinet · Y. Lebreton · A. Miglio · J. Montalbán · M.J.P.F.G. Monteiro · J. Provost · I.W. Roxburgh · R. Scuflaire · J.C. Suárez · M. Suran

$\ell = 0$ Frequencies



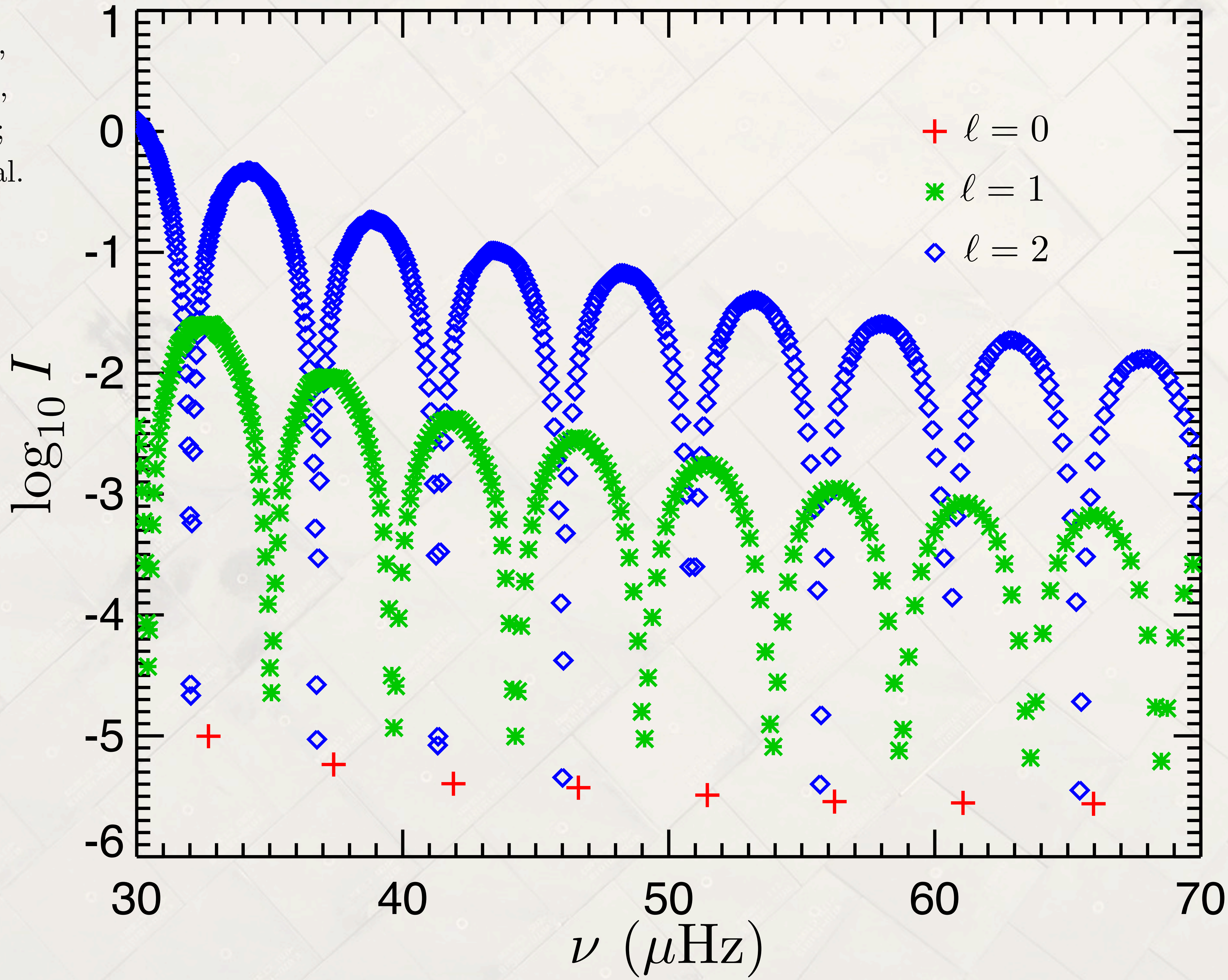
$\ell = 0, 2$ Small Separation



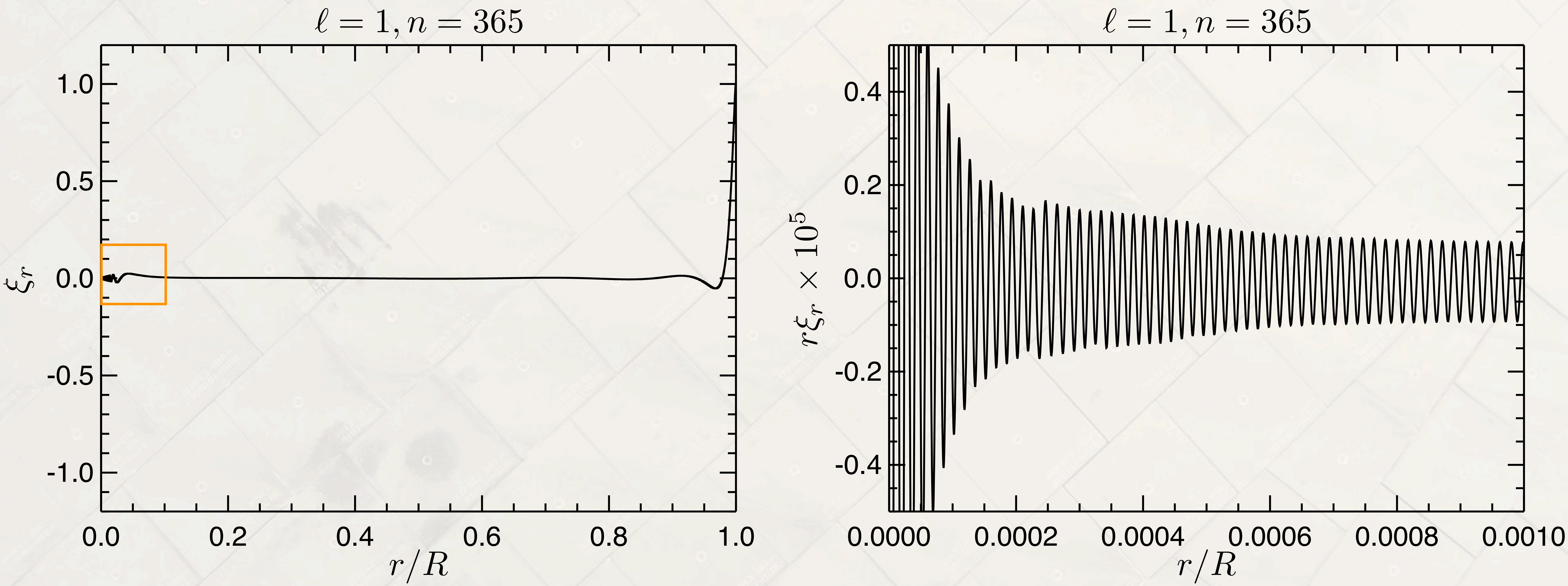
In all cases, departures from ESTA results are small

g-mode inertias in a red giant model

M = 2.0 M$_\odot$,
R = 11.0 R$_\odot$,
L = 57.8 L$_\odot$;
cf. Dupret et al.
(2009)

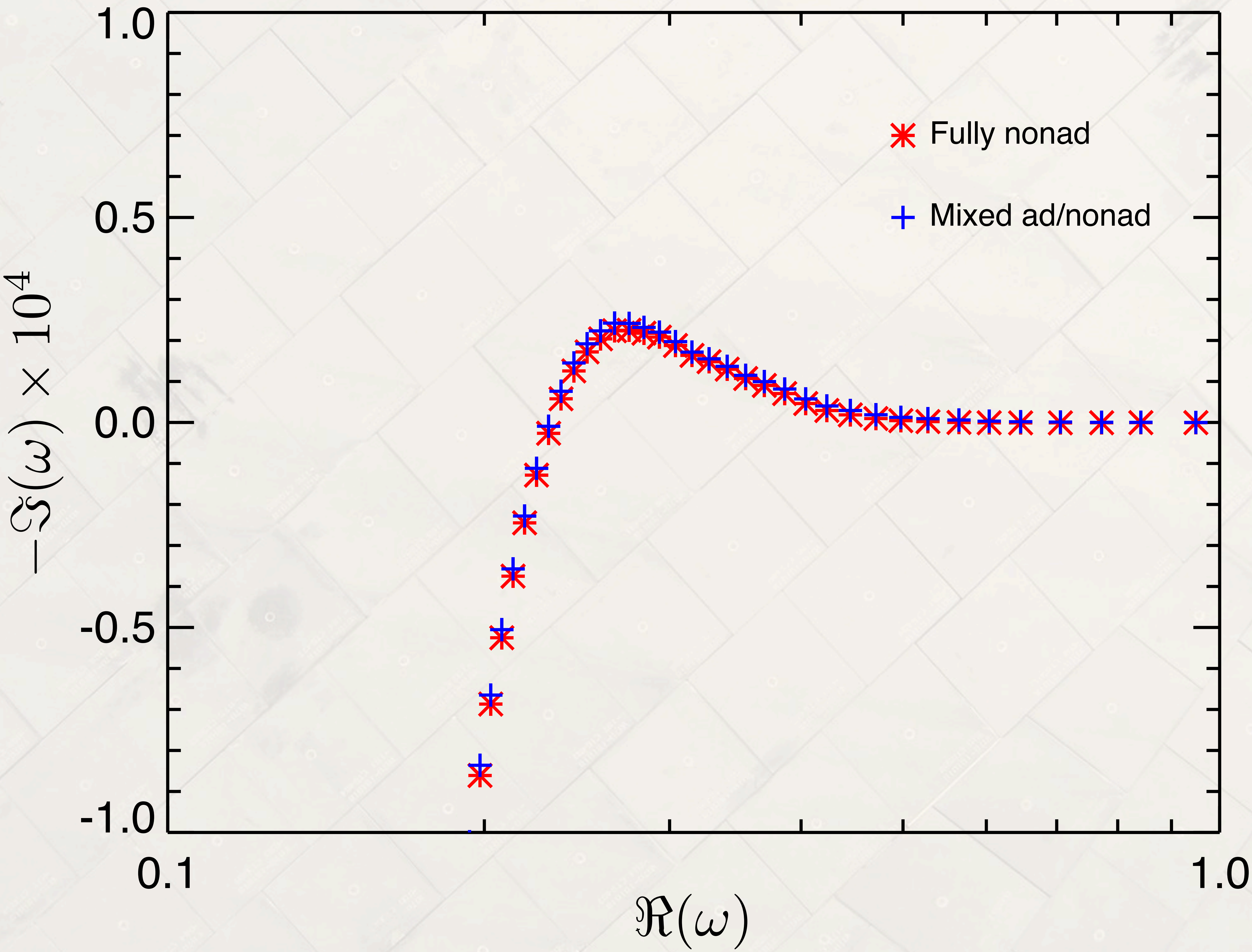


Example eigenfunction of the red giant model



The Magnus method readily handles the highly oscillatory eigenfunctions in the stellar core

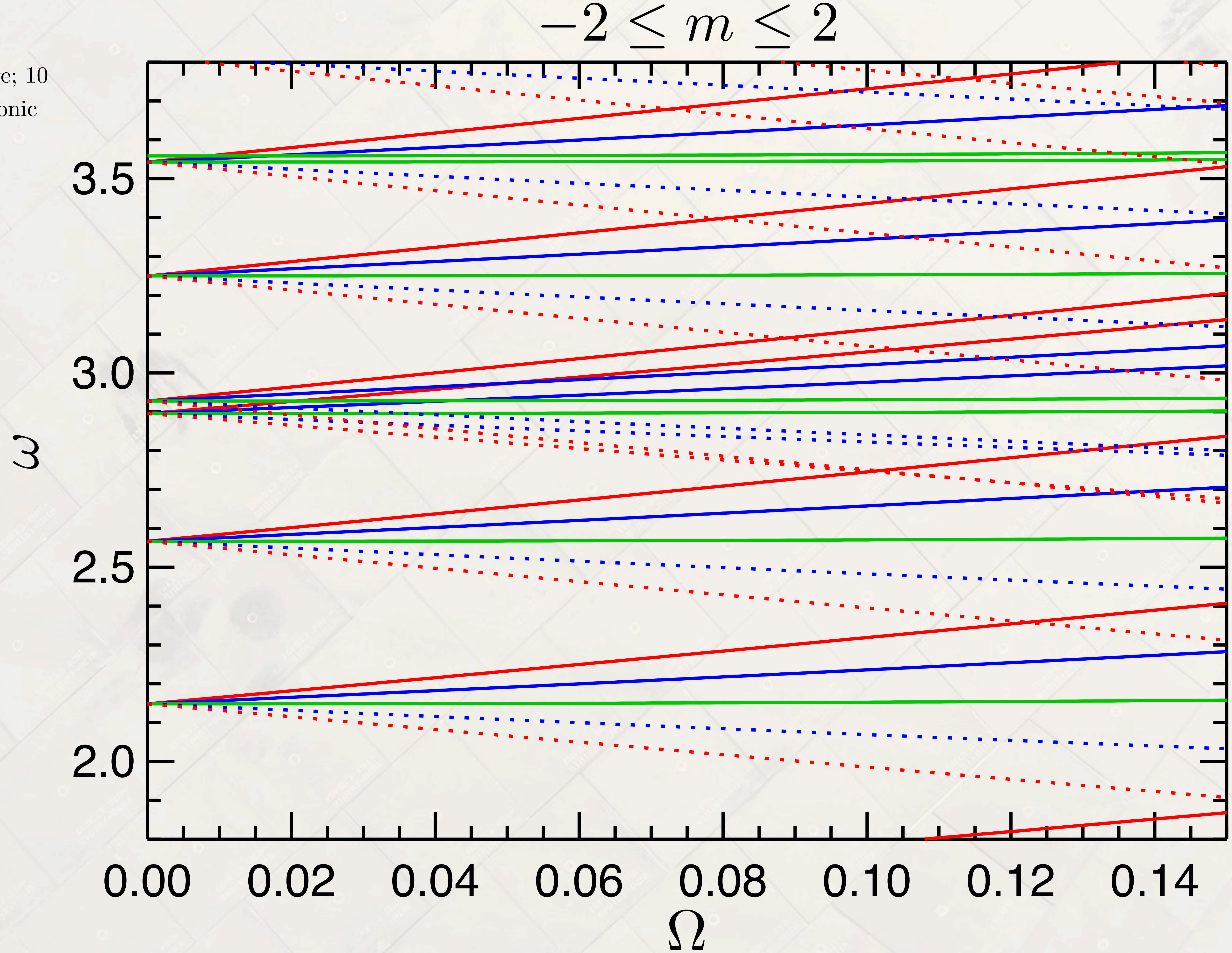
Nonadiabatic eigenfrequencies for a mid-B type star



The mixed adiabatic/nonadiabatic approach is numerically more robust, without sacrificing accuracy

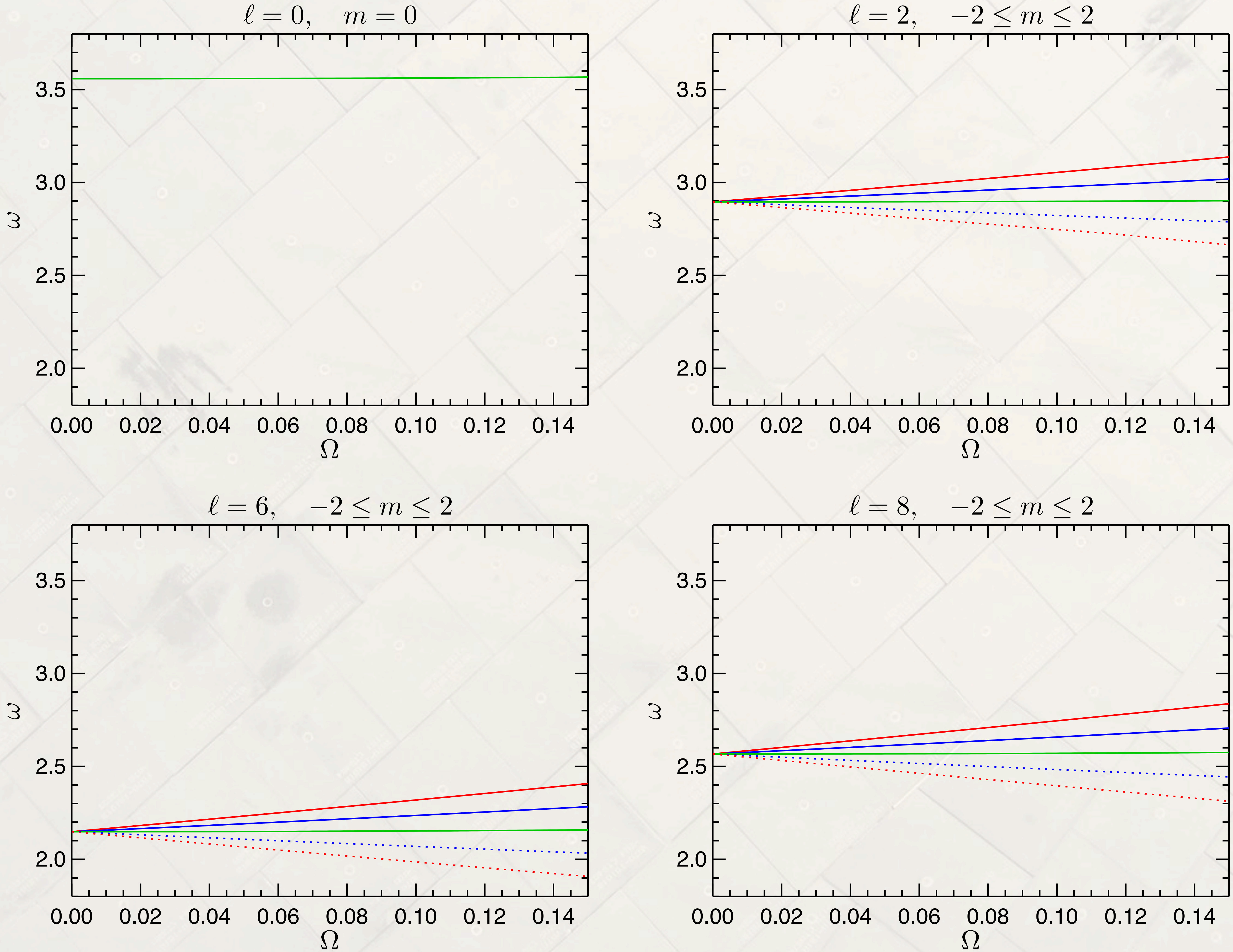
Rotational splitting in the $n = 0$ polytrope

Non-perturbative; 10 spherical harmonic terms



Modes with $\ell = 0, 2, 4, \ldots$ all appear together

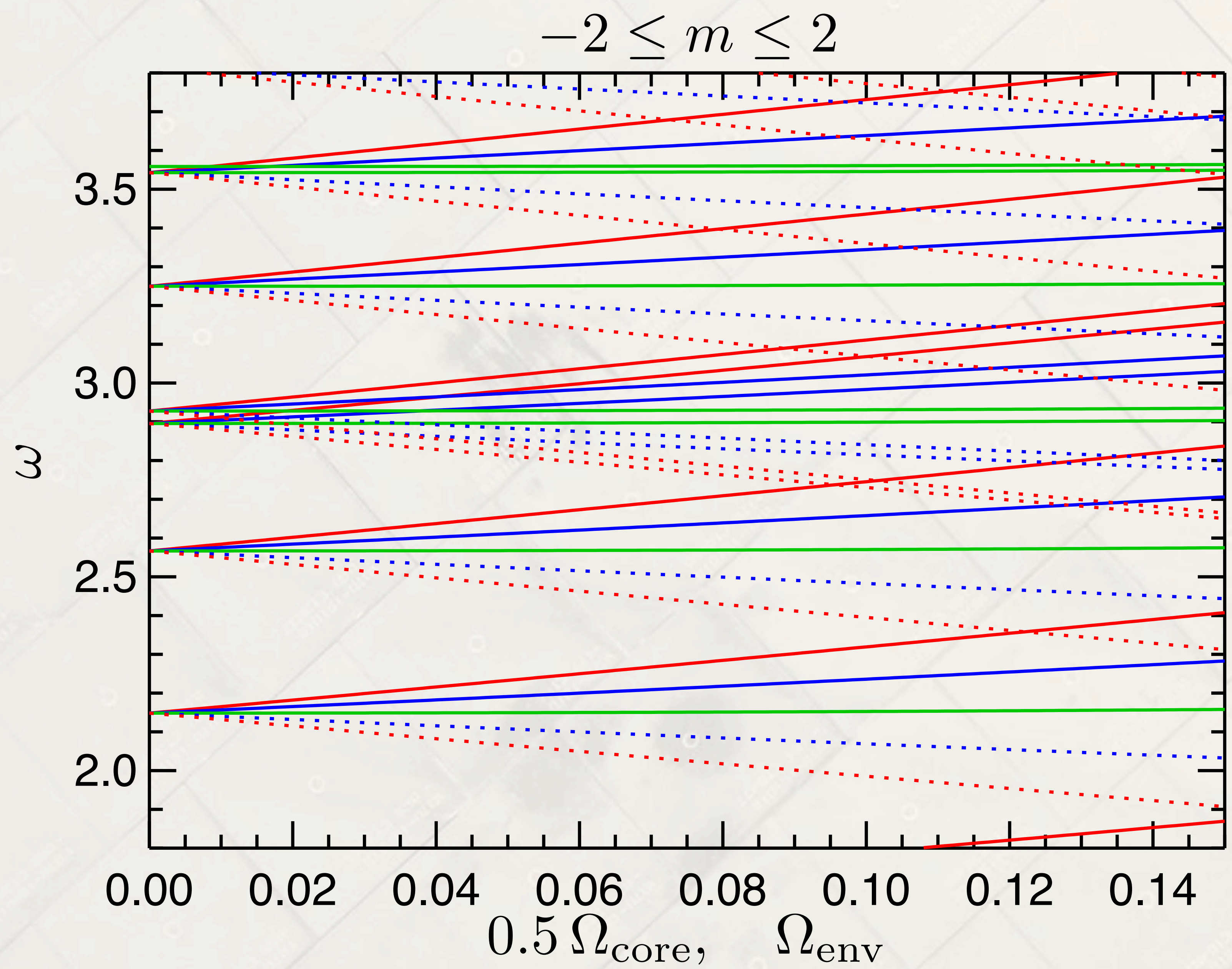
Rotational splitting: Cleaning up the mess



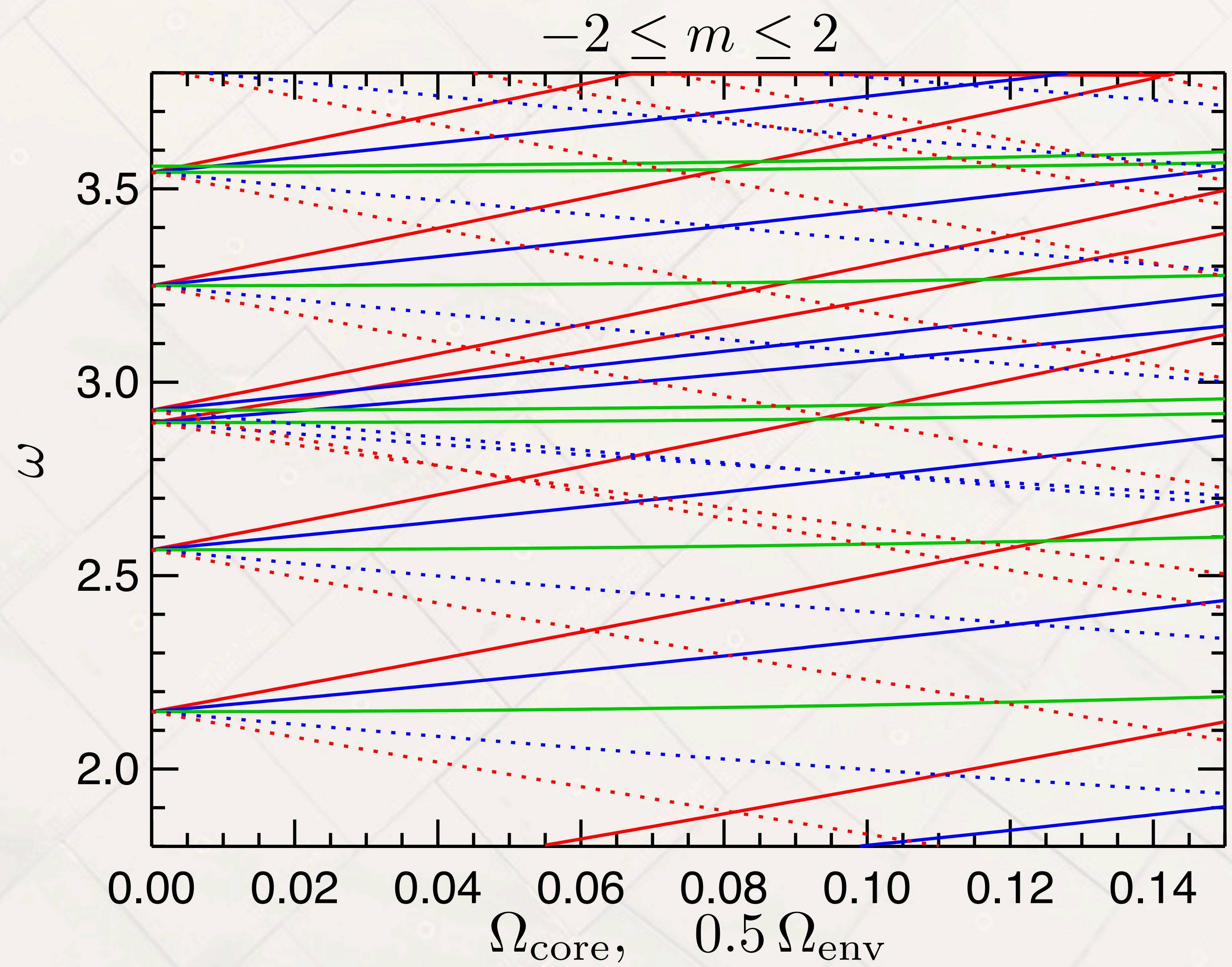
<u>Mode tracking uses the fact that mode frequencies evolve continuously with Ω</u>

Differential rotation: the $n = 0$ polytrope with core/envelope shear

Fast core

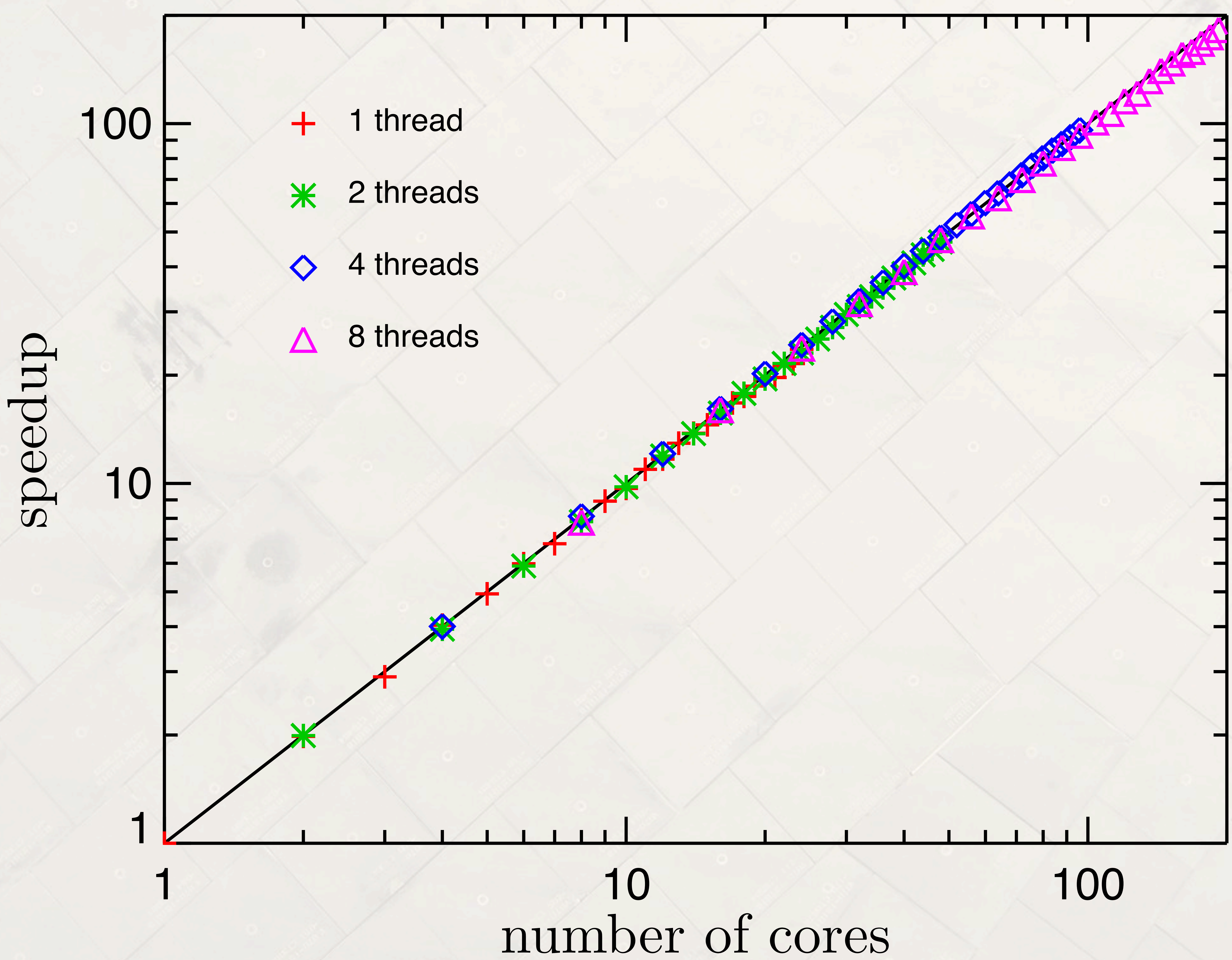


Fast envelope



Simple explanation: the modes are mainly trapped in the envelope

Benchmarking the parallel performance of GYRE



The future of GYRE

- Upcoming improvements
  - implement post-processing (e.g., mode inertias, work functions)
  - combine nonadiabatic & differential rotation functionality
  - add centrifugal force, departures from sphericity
- A full description of the code will appear in a forthcoming paper
- Scheduled for open-source release mid-2013
- Pre-release access on request