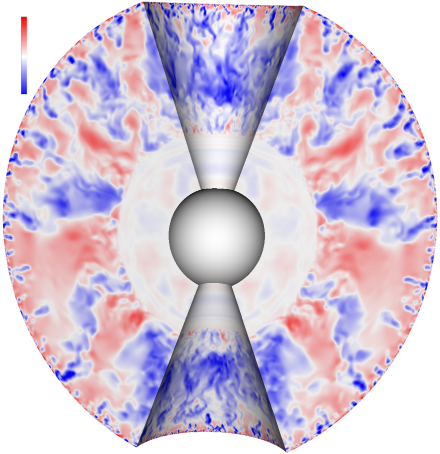
Georgia State University
Physics and Astronomy

OVERSHOOTING, FILLING FACTORS, AND PLUME DYNAMICS

with the MUltidimensional Stellar Implicit Code (MUSIC)



ChalCA V, November 8, 2023

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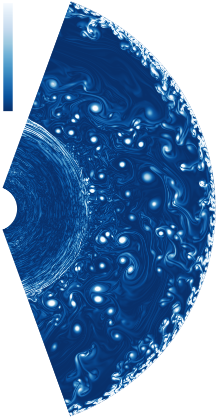
Thanks to my collaborators:
J. Pratt (GSU), I. Baraffe (Exeter, ENS de Lyon), and the MUSIC developers group

OUTLINE

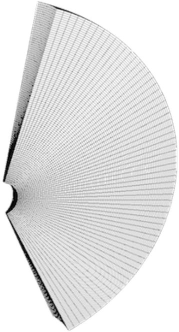
- We study realistic global simulations of stars in 2D and 3D using the MUlti-dimensional Stellar Implicit Code (MUSIC), developed in Isabelle Baraffe's group at the University of Exeter.
- We will begin by describing the numerical methods in this code that allow us to produce a long time series of data (in 2D typically we examine ~ 100 convective turnover times).
- We then use this simulation data to examine convection, overshooting, and the filling factor.
- The overshooting depth has been theoretically linked to a filling factor for convection (e.g. Zahn 1991).
- We investigate two common definitions of the filling factor to understand whether they do correlate with overshooting depth.
- We describe a new parameter that correlates with the overshooting depth: the "plume interaction parameter".



Visualization: Vorticity in a $1\,M_\odot$ pre-main sequence star, simulated with the MUSIC code.

THE FULLY COMPRESSIBLE FLUID EQUATIONS SOLVED BY MUSIC

Compressible hydrodynamic equations for convection include density ρ, momentum $\rho\vec{u}$, and internal energy ρe:



grid used in shell wedge simulations with MUSIC.

$$\frac{\partial}{\partial t}\rho = -\nabla\cdot(\rho\mathbf{u}) \quad (1)$$

$$\frac{\partial}{\partial t}\rho\mathbf{u} = -\nabla\cdot(\rho\mathbf{uu}) - \nabla\mathbf{p} + \rho\mathbf{g} \quad (2)$$

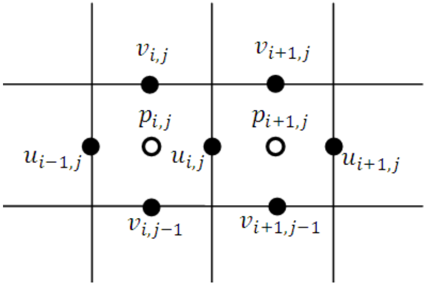
$$\frac{\partial}{\partial t}\rho e = -\nabla\cdot(\rho e\mathbf{u}) + \mathbf{p}\nabla\cdot\mathbf{u} + \nabla\cdot(\chi\nabla\mathbf{T})\,. \quad (3)$$

- The thermal conductivity χ is calculated from a realistic opacity for a star.
- We have numerical viscosity, but no explicit viscosity and no subgrid scale model $\rightarrow$ implicit Large Eddy Simulation.

FINITE VOLUME METHOD

- Staggered grid: scalars are located at cell centers, but velocity components are located at cell boundaries
- Physical quantities are interpolated to grid interfaces using a monotone upwind scheme for conservation laws (MUSCL) method.
- Linear reconstruction of variables is limited with a van Leer limiter (1974).
- The resulting finite volume method is second-order accurate in space, total variation diminishing (TVD).

velocity $= \langle u, v \rangle$



IMPLICIT TIME INTEGRATION

- The system of equations is discretized with the Crank-Nicholson scheme (second order).
- Low-storage Jacobian-free Newton Krylov (JFNK) solver, fully implicit time integration. (Knoll & Keyes JCP 2004.)
- We use a physics-based preconditioner, obtained from a low-accuracy semi-implicit solution of our matrix.
- In practice both the preconditioning and JFNK time integration are taken care of by the Trilinos library (Sandia National Labs, US).

Courant-Friedrichs-Lewy (CFL) numbers for fluid advection, stiff acoustic waves, and radiative diffusion:

$$\begin{aligned} \mathrm{C}_{\mathrm{adv}} &= \Delta t \, \mathrm{max}(|u|/\Delta x) \\ \mathrm{C}_{\mathrm{hydro}} &= \Delta t \, \mathrm{max}((|u| + c_s)/\Delta x) \\ \mathrm{C}_{\mathrm{rad}} &= \Delta t \, \mathrm{max}(k_{\mathrm{rad}}/\rho c_p \Delta x^2) \end{aligned}$$

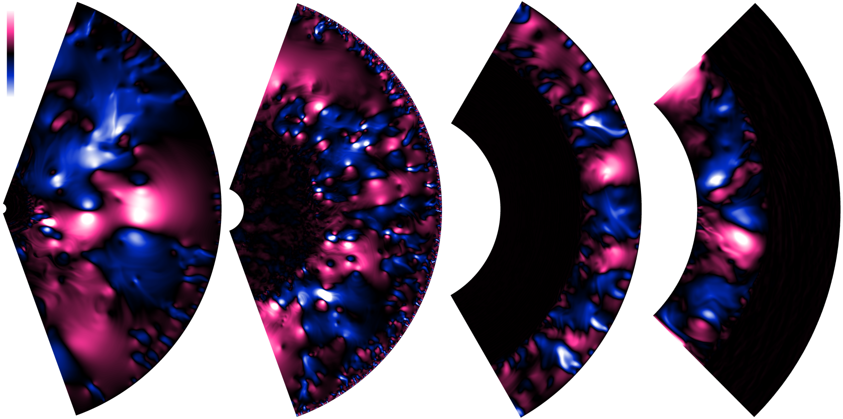
These can be combined to produce a Mach number:

$$\mathrm{M}_{\mathrm{s}} \sim \mathrm{C}_{\mathrm{adv}}/(\mathrm{C}_{\mathrm{hydro}} - \mathrm{C}_{\mathrm{adv}})$$

DETAILS OF THE JACOBIAN FREE NEWTON KRYLOV SOLVER

- JFNK methods use nested iteration at each time step:
    1. loop for Newton-Raphson iterations
    2. loop over Krylov subspace (GMRES)
    3. loop to determine preconditioner (GMRES)
- A physics-based preconditioning matrix is a solution to our physical system, calculated using an efficient but comparatively inaccurate semi-implicit scheme (acoustic waves and thermal diffusion are treated implicitly, and advection is treated explicitly).
- Linear iterative method on the inside (loop 3). Picard linearization is used. Linearization errors in calculating the preconditioner should not affect the ultimate solution.
- Nonlinear iterative method on the outside (loop 1), low error compared to semi-implicit methods.
- In practice all of the time integration is taken care of by the Trilinos library (Sandia National Labs, US).

MUSIC SIMULATIONS OF STELLAR CONVECTION



Radial velocities in MUSIC simulations of stars at different evolutionary stages, from left to right: $3M_\odot$ RGB star, $1M_\odot$ PMS sun, $1M_\odot$ MS star, and a $20M_\odot$ MS star. Outward flows are indicated in pink, while inward flows are in blue; the zero point is black.

SIMULATING STELLAR CONVECTION: 2D VS. 3D

- We simulate each star in both 2D and 3D using identical simulations (except for the dimensionality).
- For all pairs we simulate, 2D time-averaged velocities are somewhat higher, and overshooting depth is similar fairly similar in 2D and 3D (e.g. Pratt et al 2020).
- The filling factor has been theoretically linked to overshooting depth. If that link is clear, it could compensate for the higher 2D velocities.

How do we calculate the filling factor, and is it different at the convective boundary for 2D and 3D simulations?

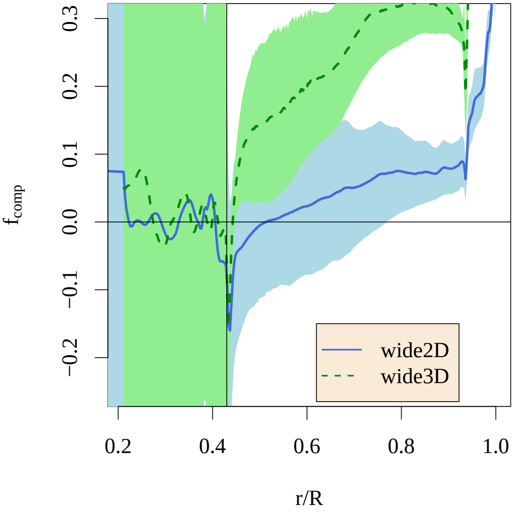
A FILLING FACTOR BASED ON THE CONVECTIVE FLUX

- Following Zahn 1991, we calculate a filling factor based on the convective flux:

$$f(r,t) = \frac{\overline{u_r(r,\theta,t)\,T_1(r,\theta,t)}}{u'_{r,\mathrm{RMS}}(r,t)\,T'_{1,\mathrm{RMS}}(r,t)}$$

  Here the prime means that the RMS is calculated only for inflows. The bar indicates an average in the angular direction.

- This expression for the filling factor is negative at the CB in all of our simulations, because the convective flux is also negative there.
- Complex boundary layer type flows appear to contaminate this measure.
- We look at time averages taken over long times (line=average, shaded area=one standard deviation).

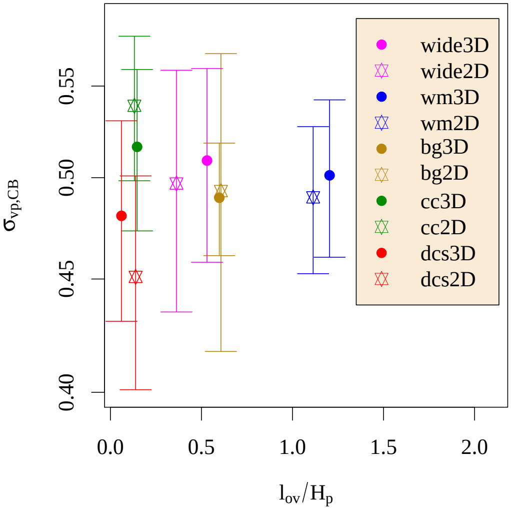


A FILLING FACTOR BASED ON THE VOLUME PERCENTAGE OF INFLOWS

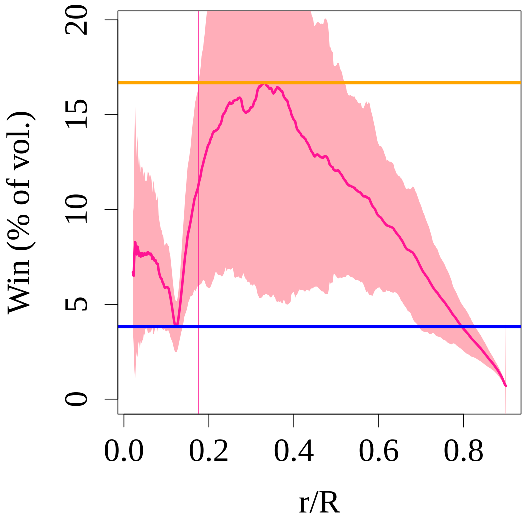
- This definition of a filling factor is much more widely used:

$$\sigma_{\text{vp}} = \frac{V_{\text{inflow}}}{V_{\text{total}}}$$

- Although the values of σ_{vp} vary throughout the stellar radius, they are close to $1/2$ at the convective boundary for all of the simulations we examine.
- The value of $\sigma_{\text{vp,CB}}$ does not correlate with the overshooting depth we measure in our simulations.

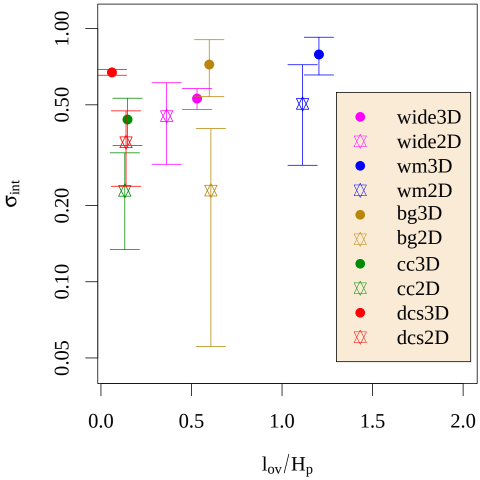


WHAT DOES CORRELATE WITH OVERSHOOTING DEPTH?



- We start by examining the (horizontally-average) width of plumes.
- This also provides us with the number of points where inflowing and outflowing plumes interact!
- In all of the convection zones we simulate, the time-averaged radial profile of the average width has a characteristic shape.
- W_{CZ} = peak of time-averaged plume width in the middle of the convection zone.
- W_{OL} = minimum of time-averaged plume width just beyond the convective boundary.

PLUME INTERACTION PARAMETER



- Using these maxima and minima, we define a non-dimensional ratio: $\sigma_{\text{int}} = W_{\text{OL}} / W_{\text{CZ}}$
- We call this the ‘plume interaction parameter’.
- This parameter is always larger in for 3D simulations (dots) than 2D simulations (stars) for all of our simulations.
- In systematic comparisons (e.g. of stars of different mass) we also find that the plume interaction parameter correlates well with overshooting depth. Further parameter studies are needed (current ongoing work!).

SUMMARY

- The implicit time integration at the core of the MUSIC code allows us to simulate over long windows of stellar convection. This makes it easier to study meaningful statistics.
- When we evaluate them at (or near) the convective boundary, neither a filling factor based on the convective flux, nor a filling factor based on the volume percentage correlates with overshooting depth.
- We are studying a new quantity, the plume interaction parameter. This parameter shows clear differences between 2D and 3D simulations.
- We are currently working on a paper to describe these ideas in full detail: Dethero et al., in prep., 2023. (Stay tuned!)

Thank You!

THERMAL CONDUCTIVITY AND OPACITY

- The thermal conductivity is related to the temperature and density: $\chi = 16\sigma T^3/3\kappa\rho$.
- σ is the Stefan-Boltzmann constant, from the Stefan-Boltzmann law for black body radiation $\ell = \sigma T^4$ (ℓ is energy radiated per surface area).
- Opacity: absorption and scattering of radiation in a medium.
- κ is the Rossland opacity: average opacity (absorption and scattering of radiation in a medium) weighted with a temperature derivative of the Planck distribution.
- Rossland opacity is valid when the plasma is locally in thermal equilibrium – a good approximation for an optically thick medium like a stellar plasma.
- For the range of temperatures in our stellar simulations, we use tables produced by the Opacity Project at Livermore (OPAL), which are identical to the tables used in MESA to produce the stellar structures.

EQUATION OF STATE

- A typical equation of state for hydrodynamic simulation is: $\vec{P} = (\gamma - 1)\rho e$, where $\gamma = c_p/c_V = 5/3$ and e is the specific internal energy.
- In a star γ varies due to partial ionization and radiation pressure.
- The degree of ionization is high in the core, but decreases as the surface of the star is approached.
- 1D stellar evolution calculations typically take this into account. Our goal is to do this similarly accurately.
- Pressure $p(\rho, e)$ and temperature $T(\rho, e)$ are interpolated from a tabulated equation of state.
- The tables we use for the equation of state assume: inter-particle forces can be neglected, partial ionization, electron degeneracy, realistic chemical mix for the sun: H, He, C, N, O, Ne, Mg, Si.