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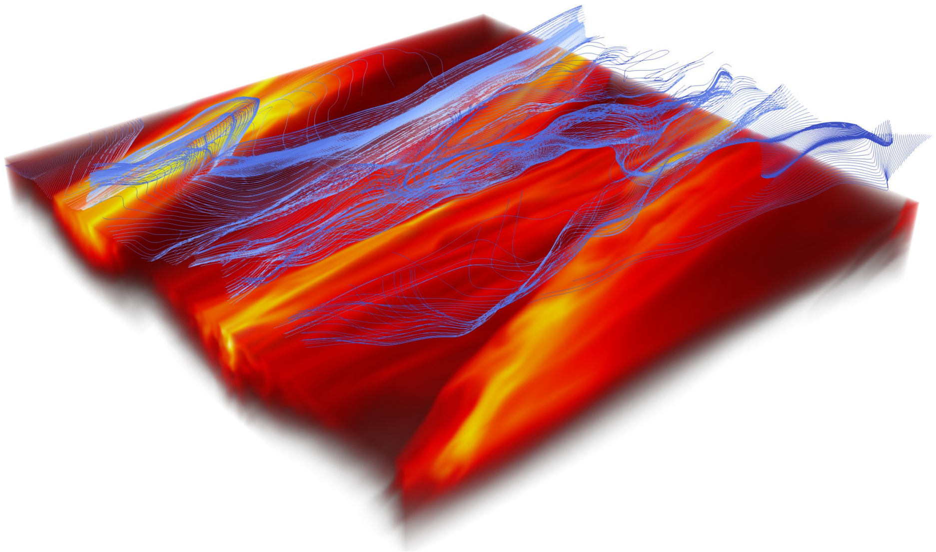
# An efficient spectral Poisson solver for NIRVANA-III: the shearing-box case with vertical vacuum boundary conditions



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# Introduction

Self-gravity (SG) crucial in astrophysics: cloud collapse, FU Orionis outbursts, Gravitational Instability, gravito-turbulent dynamos etc.

→ Necessary to solve Poisson equation: $\Delta\phi = 4\pi G\rho$

## Spectral method

Solve Poisson Eq. in Fourier space, $\hat{\Phi}(\boldsymbol{k}) = -\frac{4\pi G\,\hat{\rho}}{||\boldsymbol{k}||^2}$ followed by an inverse transform

**Pros:** very accurate, efficient thanks to FFT algorithms, timings are problem independent

**Cons:** Unrealistic domain repetitions and average of source term in num. box should be 0 (Mandal et al. 2023)

# Introduction

Solve Poisson Eq. **efficiently**, with **high accuracy** and **realistic boundary conditions** (free BC) in uniform cartesian grids ?

Vico, Greengard & Ferrando 2016 (VGF) method (from plasma and condensed matter phys.) modifies the Green's function in Fourier space to account for free-BC.

**VGF-HybridBC**: a novel full spectral method, based on the VGF method, designed to handle **mixed periodic and vacuum boundary conditions** in **shearing boxes**

# General description in shearing boxes

Three steps:

1. Domain made fully periodic by performing a coordinate transformation (Gressel & Ziegler 2007, Johansen et al. 2009).
2. The Poisson equation is solved in the new periodic reference frame using the spectral method (see the section below).
3. Potential mapped back to the initial coordinate system.

**We focus only on step 2 for solving Poisson equation with two periodic BC and one free BC.**

# The revisited VGF-HybridBC method

$$\hat{\mathcal{G}}^L(k, k_z) = -\frac{1}{k^2 + k_z^2}$$

**Periodic boundary conditions**

$\longrightarrow$

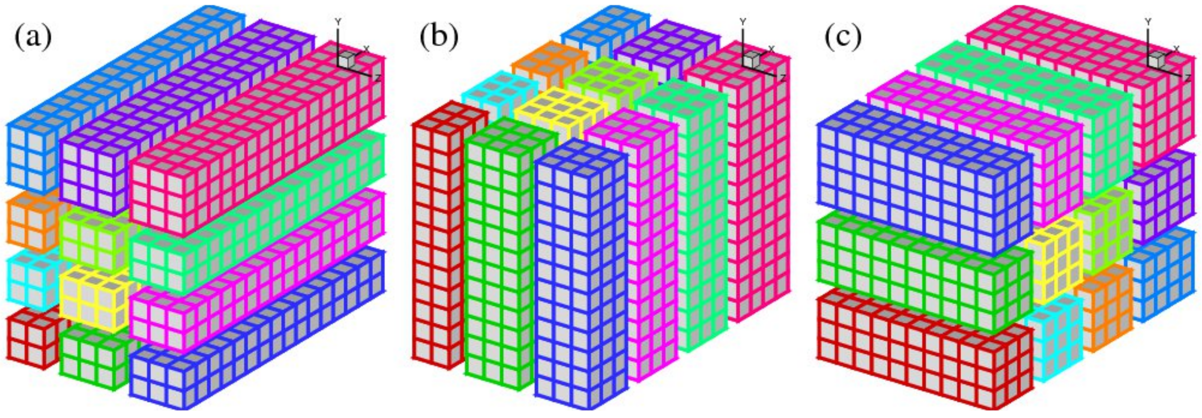
$$\hat{\mathcal{G}}^L(k, k_z) = \begin{cases} L^2/2 \\ \dfrac{\left[k_z L \sin(k_z L) + \cos(k_z L) - 1\right]}{k_z^2} \\ -\dfrac{e^{-kL}\left(\frac{k_z}{k}\sin(k_z L) - \cos(k_z L)\right) + 1}{k^2 + k_z^2} \end{cases}$$

**Vertical open boundary conditions**

Rendon Restrepo et Gressel, 2025b, A&A (Numerical methods and codes)

# Implementation details

- Code *NIRVANA-III* (AIP)
- Librairie P3DFFT : décomp. en crayons




Li & Laizet (2010)

- Crayons = compromis performance gravité + solveur Magnétohydrodynamique **(MHD)**

- Données : zero-padding + redondance Hermitienne

# Benchmarks

## 3D test: mixed boundary conditions - $\rho(x,y,z) = \cos\left(k_x x\right)\, \cos\left(k_y y\right) e^{-\frac{1}{2}(z/H)^2}$

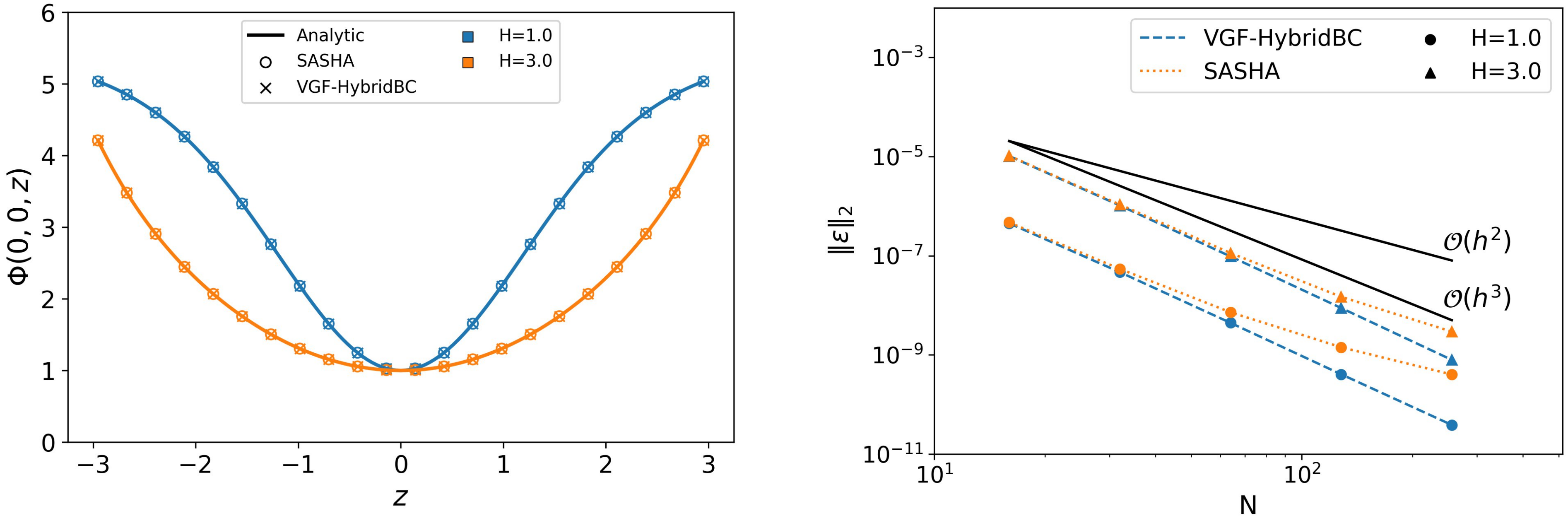



**Fig. 1.** Potential along the z direction associated with a 3D density distribution: periodic in x and y, Gaussian in the vertical direction.

*Left:* Potential. *Right:* Numerical convergence.

# Performance

Time spent in the spectral solver is less than 6% of the whole runtime.

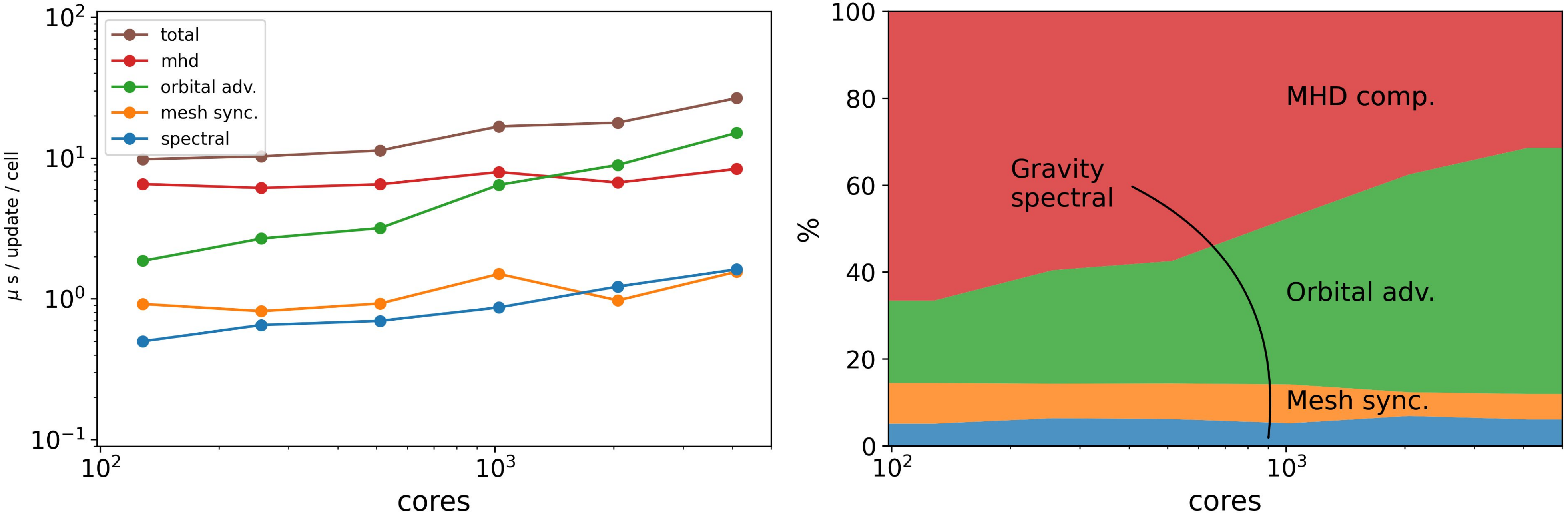
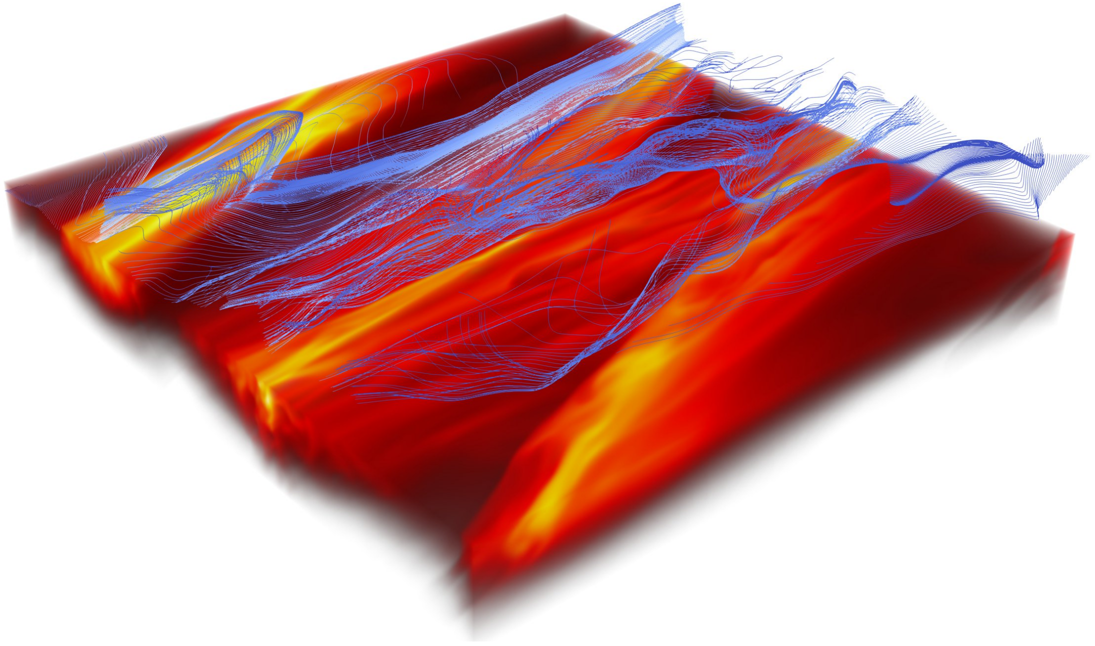



**Fig. 2.** Weak scaling study for a workload of $32^3$ cells per MPI rank and using a pencil decomposition (P3DFFT).

# Astrophysical application

## Gravito-turbulent dynamos



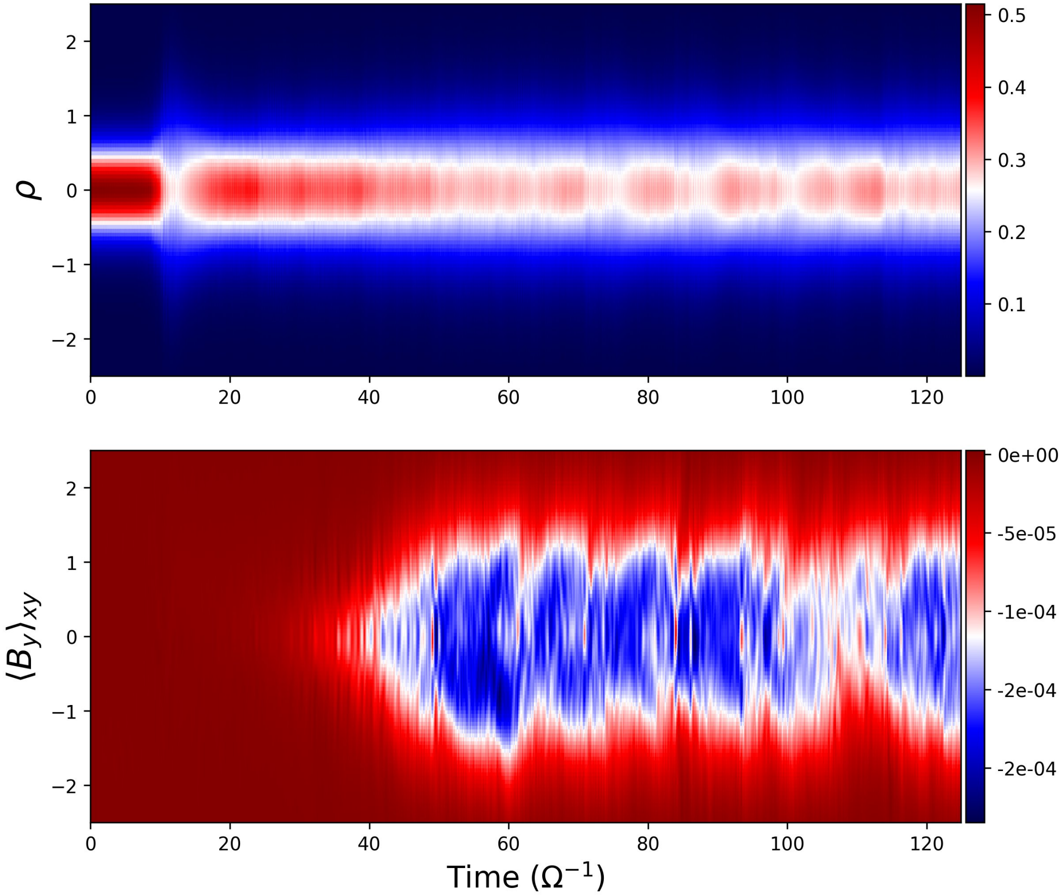



**Fig.** Magnetif field amplification in a gravito-turbulent disc

Left: Volume-rendered density (shaded) with magnetic field lines (streamlines)

Right: Dynamo effect: top: density distribution; bottom: toroidal magnetic field

# Take-home messages

- VGF adapted to shearing boxes: modify Green’s function in Fourier space for accounting correct BC
- Iimplementation thanks to P3DFFT library (pencil decomposition) = balancing load of hydro. solver and grav. spectral solver
- Third order accurate in space, very efficient thanks to FFT
- Portability: yes (provided using adapted libraries like KokkosFFT, heFFTe)

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# Danke für Ihre Aufmerksamkeit
# Merci pour votre attention
# Thank you for your attention

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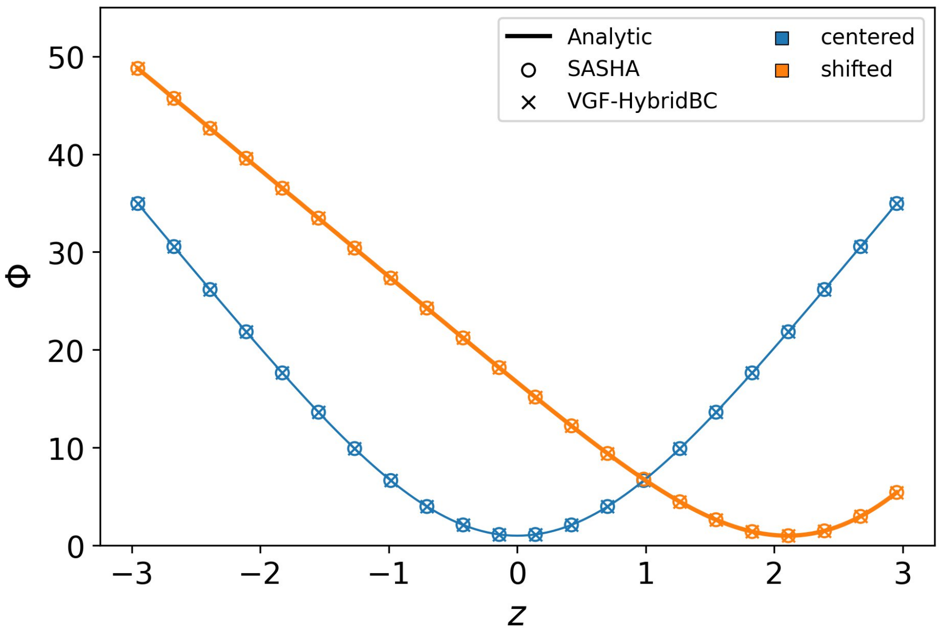
# Benchmarks

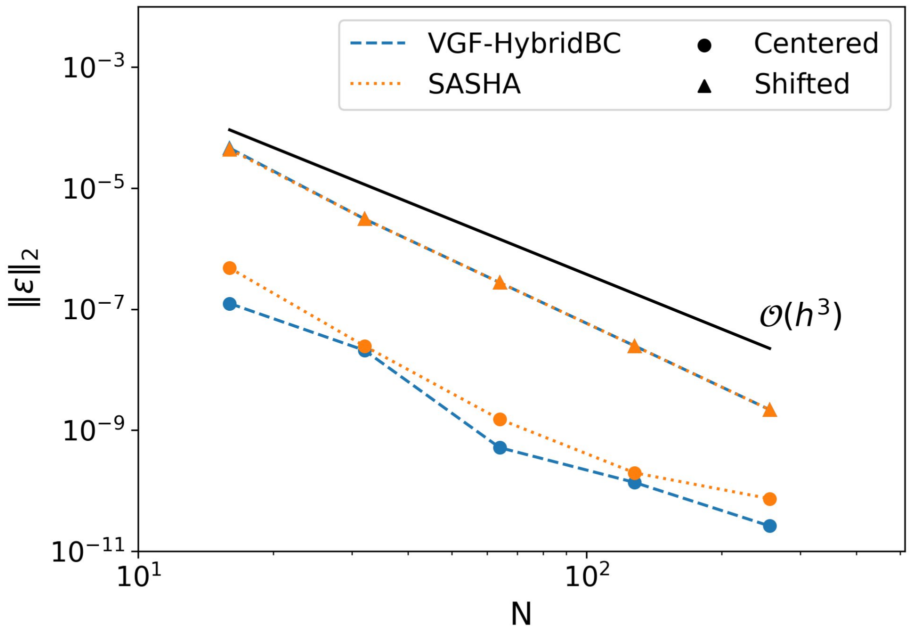
## 1D test: Gaussian density distr. with vacuum BC -

$$\rho(z) = \begin{cases} e^{-\frac{1}{2}(z-z_0)^2} & \text{if} \quad z \in [-L_z/2, L_z/2] \\ 0 & \text{else} \end{cases}$$

**Fig. 1.** Potential associated with a one-dimensional vertical Gaussian distr. We considered a profile i) centered around the midplane, and ii) a shifted profile.

*Left:* Potential.
*Right:* Numerical convergence.



# The revisited VGF-HybridBC method

Fourier transform in x, y directions :

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2} - k^2\right)\tilde{\Phi}(z) = 4\pi G\tilde{\rho}(z)$$

where: $k^2 = k_x^2 + k_y^2$

1D Helmholtz equation

The potential is simply obtained by convolution in the vertical direction:

$$\tilde{\Phi}(z) = 4\pi G \int_{-L_z/2}^{L_z/2} \mathcal{G}_k(z - z')\tilde{\rho}(z')\mathrm{d}z'$$

where $\mathcal{G}_k$ is the Green‘s function associated to above differential equation.

Our method, inspired by VGF, consists on:

**(1)** recognizing that above integral form remains unchanged in a finite-sized box if the Green’s function is replaced by:

$$\mathcal{G}^L(z - z') = \mathrm{rect}\left(\frac{z - z'}{2L}\right)\mathcal{G}_k(z - z')$$

where $\mathrm{L} = \alpha L_z$ is a suitable enclosure ($\alpha > 1$)

**(2)** computing the Fourier transform of this new Green's function in the vertical direction

# Comparison with other methods

Koyama & Ostriker (2009)

(Implemented in Athena)

Full FFT method that requires 4 steps:

1. in-plane Fourier transform,

2. modifcation of the density in the mirror regions and vertical FFT,

3. Convolution

4. Backward 3D transform

The decomposition of the 3D FFT in two distinct FFTs prevents the use  of parallel three dimensional FFT, hindering the use of P3DFFT and therefore limiting the performance.

Riols, Latter, Paardekooper (2017)

(Implemented in Pluto)

1. FFT in 2D
2. Discretize and solve for each k:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2} - k^2\right)\tilde{\Phi}(z) = 4\pi G\tilde{\rho}(z)$$

3. Backward 2D transform

Their method requires to assign vertical BC.

They impose low density conditions (makes sense in stratified discs but it is not the most general)