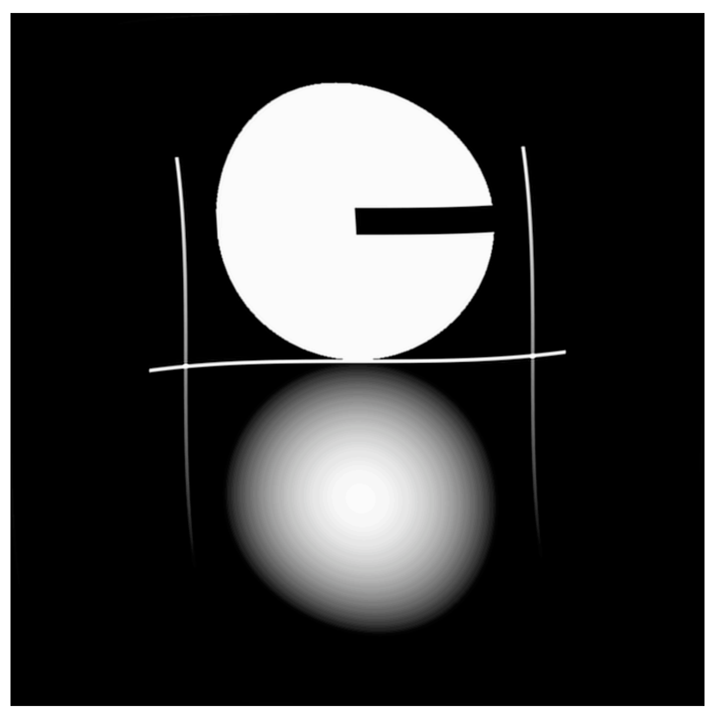
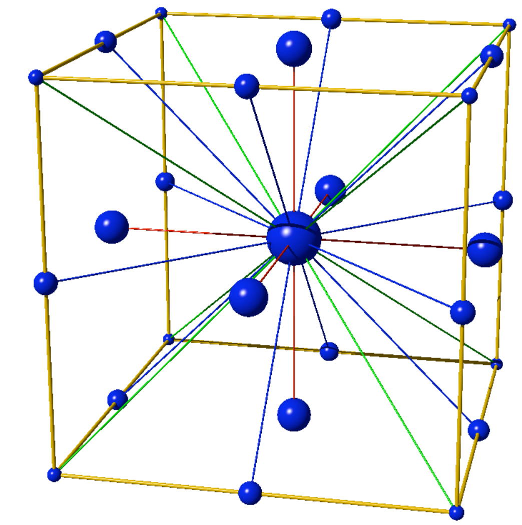
The ~~Lattice~~ Magic Boltzmann Method



Lattice Boltzmann: secret ingredients



$$Kn(Ma\partial_t f + v_x\partial_x f + v_y\partial_y f + v_z\partial_z f) = \Omega(f)$$

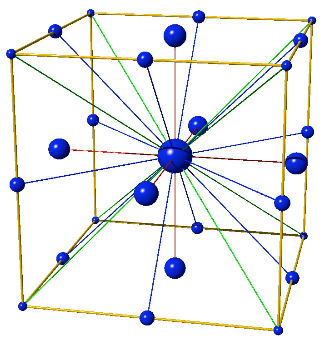
Analysis   Modeling

$$Kn(Ma\partial_t \pi_\alpha + \partial_x \pi_{\alpha x} + \partial_y \pi_{\alpha y} + \partial_z \pi_{\alpha z}) = \omega_\alpha(\pi_\alpha^{at} - \pi_\alpha)$$

ω_α : magic relaxation rates

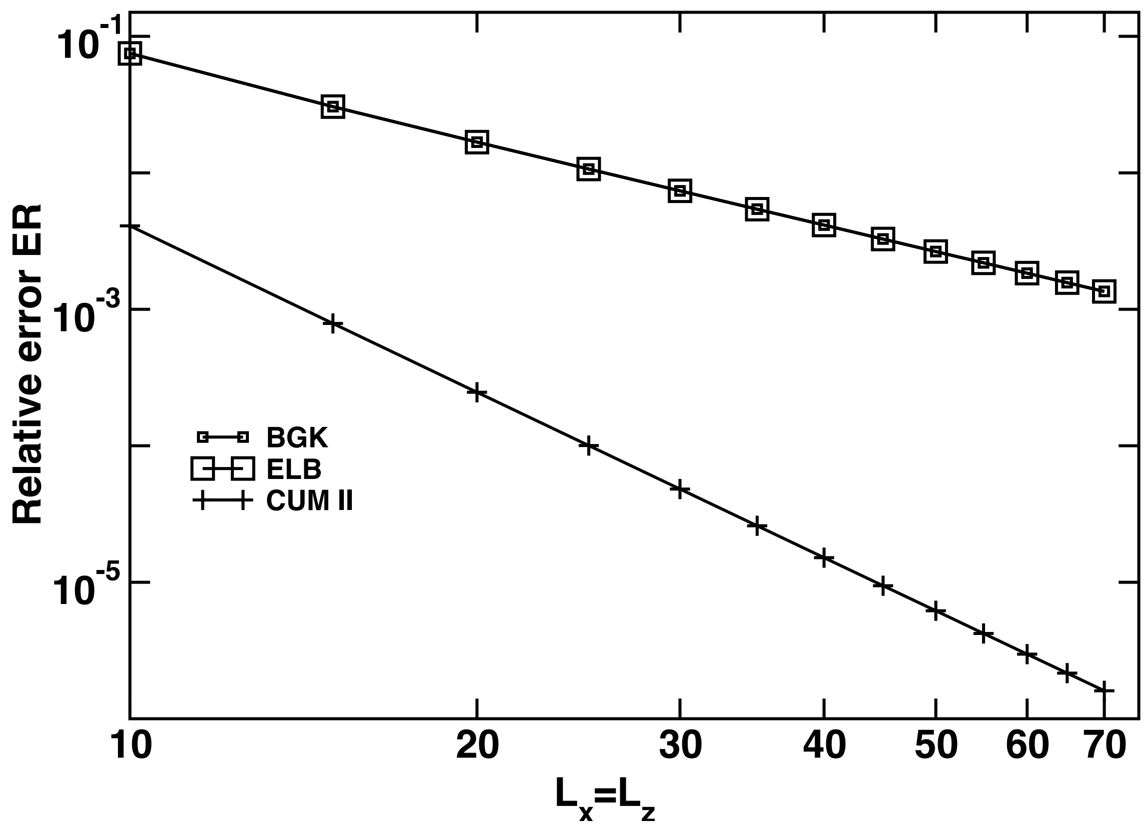
π_α^{at} : magic attractors

Cumulant method: a magic example



- D3Q27 lattice
- Magic attractors: relax **cumulants**
- Magic relaxation rate:

$$\omega_{xyz} = 2 - \omega_{xy}$$



Error in viscosity
Magic cumulant method $O(k^4)$
BGK/ELB $O(k^2)$

From Magic to Science

- Step 1: Galilean invariance
  - Central moments or cumulants
- Step 2: Optimize relaxation rates
  - Errors from Taylor analysis
  - Find roots of error pre-factors

still to be done

Galilean invariance

in weak sense

- Problem: relaxation of (raw) moments with *different* rates like in MRT method breaks Galilean invariance

Galilean invariance

in weak sense

- Regard MRT raw moment equations:

$$Kn(Ma\partial_t\pi_{xy}+\partial_x\pi_{xxy}+\partial_y\pi_{xyy})=\omega_{xy}(\pi_{xy}^{eq}-\pi_{xy})$$
$$Kn(Ma\partial_t\pi_{xx}+\partial_x\pi_{xxx}+\partial_y\pi_{xxy})=\omega_{xx}(\pi_{xx}^{eq}-\pi_{xx})$$
$$Kn(Ma\partial_t\pi_{xxy}+\partial_x\pi_{xxxy}+\partial_y\pi_{xxyy})=\omega_{xxy}(\pi_{xxy}^{eq}-\pi_{xxy})$$

- Apply Galilean transformation to 3rd eq.

$$\pi_{xx}^{eq}=\pi_x^2+1/3 \qquad \pi_x\to\pi_x+a$$
$$\pi_{xy}^{eq}=\pi_x\pi_y \qquad \pi_y\to\pi_y+b$$
$$\pi_{xxy}^{eq}=\pi_y/3 \qquad \pi_{xxy}\to\pi_{xxy}+b\pi_{xx}+2a\pi_{xy}+2ab\pi_x+a^2\pi_y+a^2b$$

$$\Rightarrow rhs_{xxy}+b\,rhs_{xx}+2a\,rhs_{xy}+2ab\,rhs_x+a^2\,rhs_y+a^2b\,rhs_0=$$
$$lhs_{xxy}+b\frac{\omega_{xxy}}{\omega_{xx}}lhs_{xx}+2a\frac{\omega_{xxy}}{\omega_{xy}}lhs_{xy}$$

Failed!

Scattering cascade

- Non-linear transformation to Galilean invariant variables
  - Central moments $\partial_{k_x}^{n_x}\partial_{k_y}^{n_y}\partial_{k_z}^{n_z}\mathbf{v}\mathcal{F}\{f\}$
  - Cumulants $\partial_{k_x}^{n_x}\partial_{k_y}^{n_y}\partial_{k_z}^{n_z}\log(\mathcal{F}\{f\})$
- Back to raw moments $\partial_{k_x}^{n_x}\partial_{k_y}^{n_y}\partial_{k_z}^{n_z}\mathcal{F}\{f\}$
  - Example 3rd moment

$$\pi_{xxy}^{at} = 2\pi_x\left(\pi_{xy} + \frac{\omega_{xy}}{\omega_{xxy}}(\pi_{xy}^{at} - \pi_{xy})\right) - 2\pi_x^2\pi_y + \pi_y\left(\pi_{xx} + \frac{\omega_{xx}}{\omega_{xxy}}(\pi_{xx}^{at} - \pi_{xx})\right)$$

Galilean invariance at 3rd order moments

in weak sense

- Perform the Galilean transformation

$$\pi_x \to \pi_x + a$$
$$\pi_y \to \pi_y + b$$
$$\pi_{xxy} \to \pi_{xxy} + b\pi_{xx} + 2a\pi_{xy} + 2ab\pi_x + a^2\pi_y + a^2 b$$

$$\boxed{\begin{aligned}\Rightarrow\ & rhs_{xxy} + b\, rhs_{xx} + 2a\, rhs_{xy} + 2ab\, rhs_x + a^2\, rhs_y + a^2 b\, rhs_0 = \\ & lhs_{xxy} + b\, lhs_{xx} + 2a\, lhs_{xy}\end{aligned}}$$

Correct!

- 3rd order moment now as Galilean invariant as they would be with BGK ansatz

Central moments versus cumulants

- Raw moments:
  - orthogonal decomposition in lattice (=arbitrary) frame of reference
- Central moments:
  - orthogonal decomposition in frame moving with flow
- Cumulants or irreducible moments
  - orthogonal decomposition in **any** frame of reference

Equilibrium central moments

- Transform to raw moments

advection for non-conserved moment!

$$\pi_{xxyz}^{at} = 2\pi_{xyz}\pi_x - \pi_{yz}\pi_x^2 + \pi_{xxz}\pi_y - 2\pi_{xz}\pi_x\pi_y + \pi_{xxy}\pi_z - 2\pi_{xy}\pi_x\pi_z - \pi_{xx}\pi_y\pi_z + 3\pi_x^2\pi_y\pi_z$$

- Central moment equilibria polynomials in first order raw moments and monomials in raw moments

Equilibrium cumulants

- Transform to raw moments

diffusion for non-conserved moment!

$$\pi^{at}_{xxyz} = -4\pi_y\pi_x\pi_{xz} + 2\pi_{xz}\pi_{xy} + 2\pi_x\pi_{xyz} + \pi_{yz}(\pi_{xx} - 2\pi_x^2) + \pi_y\pi_{xxz} + \pi_z(\pi_y(6\pi_x^2 - 2\pi_{xx}) + \pi_{xxy} - 4\pi_x\pi_{xy}))$$

- Cumulant equilibria polynomial in all lower order raw moments

Test case: 3rd order moments @ *O(Ma²)*

- Let us investigate:

$$Kn(Ma\partial_t\pi_{xyy}+\partial_x\pi_{xxyy}+\partial_y\pi_{xyyy}+\partial_z\pi_{xyyz})=\omega_{xyy}(\pi^{at}_{xyy}-\pi_{xyy})$$

- Assumptions: truncated („equilibrium“ state) at 4th order
- Expansion to low order using $\pi_{yy}=1/3+O(Ma^2)$

$$\pi_{xyy}=\pi_x/3+O(Ma^3)$$
$$\pi^{at}_{xyy}-\pi_{xyy}=O(Ma^3)$$

Test case: 3rd order moments @ $O(Ma^2)$

- Note that:

$$Ma\partial_t\pi_x = -\partial_x\pi_{xx} - \partial_y\pi_{xy} - \partial_z\pi_{xz}$$

- So:

$$\partial_x(\pi_{xxyy} - \pi_{xx}/3) + \partial_y(\pi_{xyyy} - \pi_{xy}/3) + \partial_z(\pi_{xyyz} - \pi_{xz}/3) = O(Ma^4)$$

- Hence:

$$\begin{aligned}\pi_{xxyy} &\to \pi_{xx}/3 + O(Ma^4)\\ \pi_{xyyy} &\to \pi_{xy}/3 + O(Ma^4)\\ \pi_{xyyz} &\to \pi_{xz}/3 + O(Ma^4)\end{aligned}$$

Test case: compare

Central moments	Cumulants
Failed!	
$\pi^{at}_{xxyy} = 1/9 + \pi_x^2/3 + \pi_z^2/3 + O(Ma^4)$	$\pi^{at}_{xxyy} = \pi_{xx}/3 + O(Ma^4)$
$\pi^{at}_{xyyy} = \pi_x \pi_y + O(Ma^4)$	$\pi^{at}_{xyyy} = \pi_{xy} + \pi_x \pi_y + O(Ma^4)$
$\pi^{at}_{xyyz} = \pi_x \pi_z/3 + O(Ma^4)$	$\pi^{at}_{xyyz} = \pi_{xz}/3 + O(Ma^4)$
Failed! **Failed!**	**Failed!**

Understand the errors (a research plan)

- Taylor method (Dubois) *a little modified*

$$\pi_\alpha + MaKn\partial_t\pi_\alpha + \cdots = \pi^*_\alpha - Kn(\partial_x\pi^*_{\alpha x} + \partial_y\pi^*_{\alpha y} + \partial_z\pi^*_{\alpha z})\cdots$$

Pre-collision expansion in time	=	Post-collision expansion in space

- Expansion in moment form
- Two scale parameters *several possibilities Ma & Kn suggested by Asinari*
- No generic (acoustic or diffusive) scaling

Some pitfalls on our way...

- Expansion parameters ought to be small

  Not clear for time step expansion

- Asymptotic order ought to increase with expansion

  True for Knudsen but false for Mach!

Do not forget to scale relaxation rates

$$\nu = c_s^2\left(\frac{1}{\omega_{xy}} - \frac{1}{2}\right) \Rightarrow \nu \propto Re^{-1} = \frac{Kn}{Ma} \Rightarrow \frac{1}{\omega_{xy}} = \frac{Kn}{Ma} + \frac{1}{2}$$

diffusive scaling:

Ma=Kn

better?

$$\underbrace{\pi^*_{xy}}_{} = \overbrace{\pi^{eq}_{xy}}^{O(Ma^2)} - \overbrace{\left(\frac{1}{\omega_{xy}} - 1\right)}^{O(Kn/Ma)}\left(\overbrace{Kn\partial_x\pi^*_{xxy}}^{O(Ma)!!!} + \overbrace{Kn\partial_y\pi^*_{xyy}}^{O(Ma)!!!} + \cdots\right)$$

Be careful using this: $\pi^*_{xy} = \pi^{eq}_{xy} + O(Kn)$ equilibrium as small as reminder!!!

Equilibria and their scale in Mach number

$$\pi^{eq}_{xy} = O(Ma^2)$$

$$\pi^{eq}_{xx} = O(1)$$

cyclic repetition of O(Ma), O(Ma²), & O(Ma³) for all higher order moments

$$\pi^{eq}_{xyy} = O(Ma)$$

$$\pi^{eq}_{xyz} = O(Ma^3)$$

O(Ma³) is highest order for any moment!

$$\pi^{eq}_{xxyy} = O(1)$$

no 4th order moment higher than O(Ma²)

$$\pi^{eq}_{xxyz} = O(Ma^2)$$

$$\pi^{eq}_{xxyyz} = O(Ma)$$

all odd order moments are at least O(Ma)

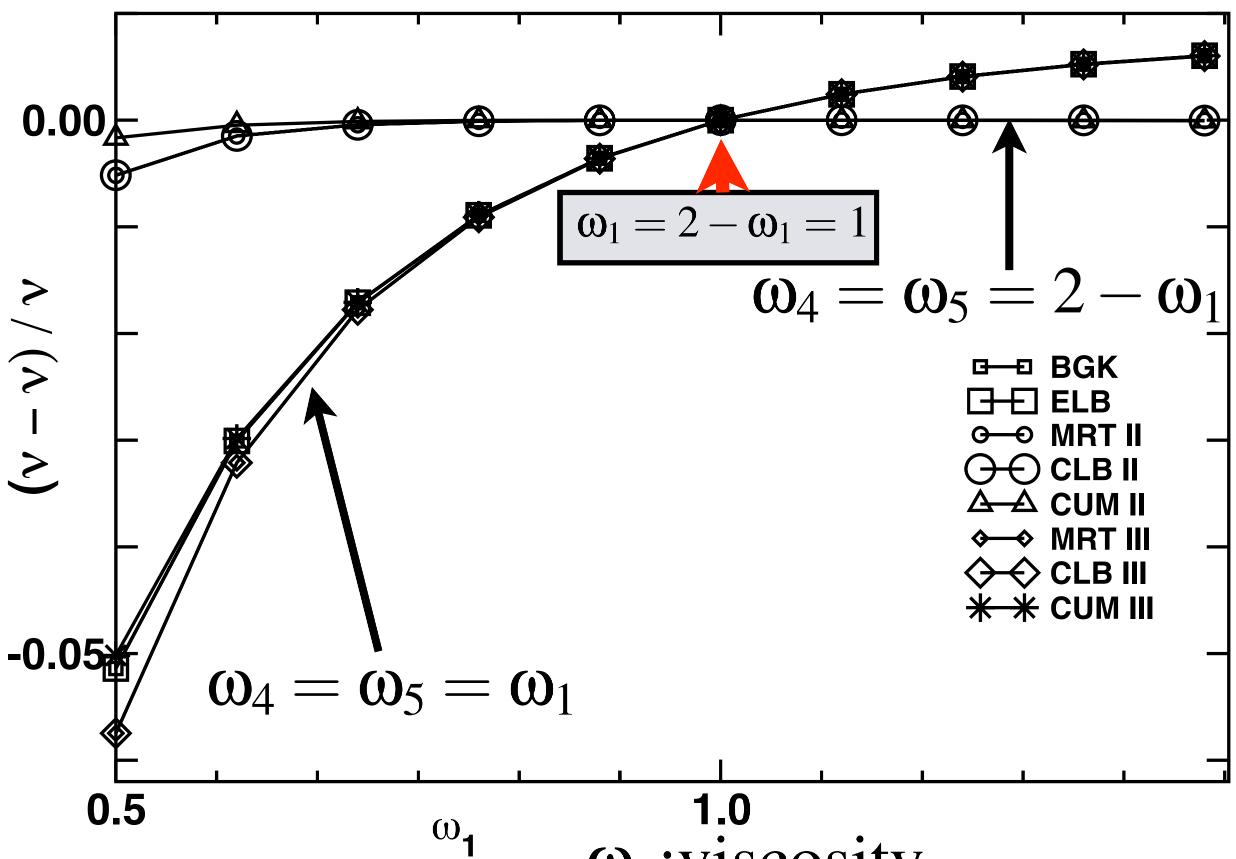
Convergence completely up to Knudsen number!

Magic parameters

Analytic solution NSE

$$u_y(x,y,z,t=0) = u_0 \sin(2x/L_x\pi)\cos(2z/L_z\pi)$$

$$u_y(x,y,z,t) = u_y(x,y,z,t=0)\, e^{-\nu t\left[\left(\frac{2\pi}{L_x}\right)^2+\left(\frac{2\pi}{L_z}\right)^2\right]}$$

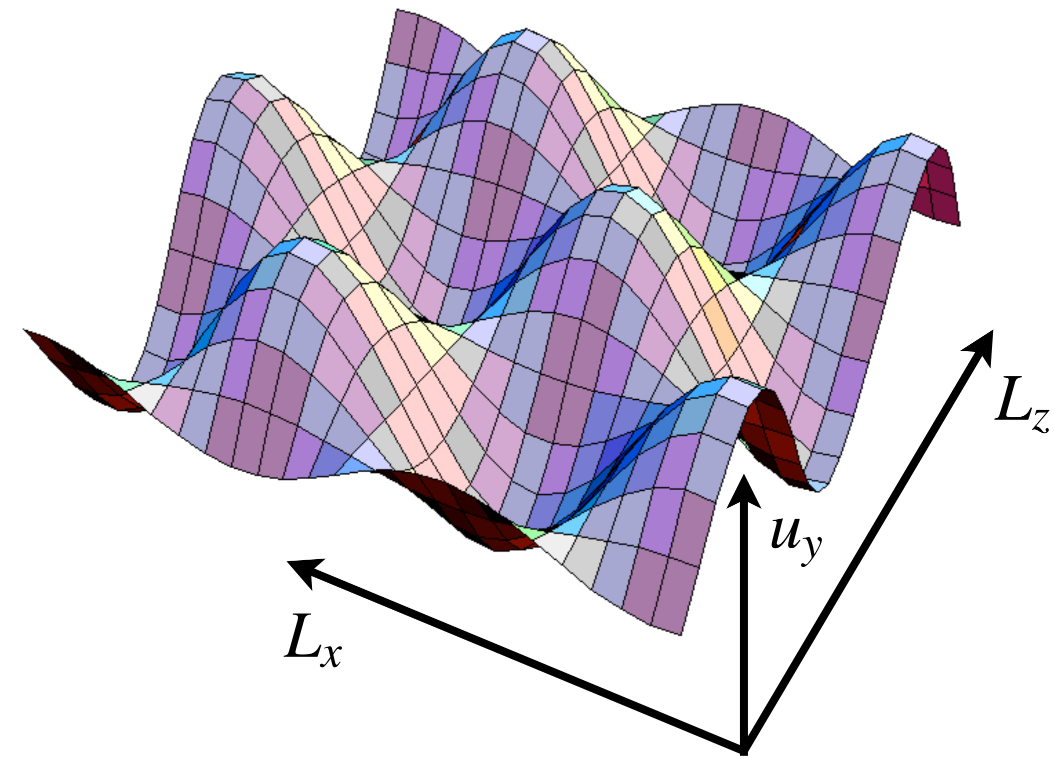


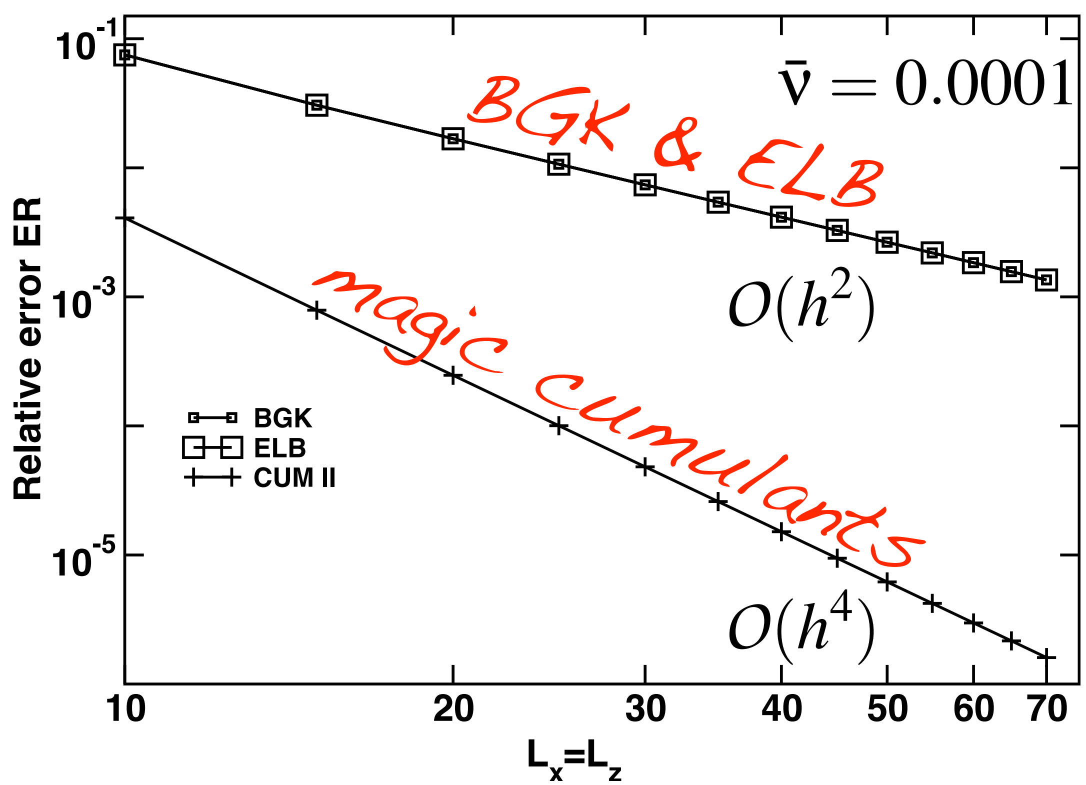
ω_1:viscosity

$\omega_3 = \omega_1 : \pi_{xxy} + \pi_{yzz}$

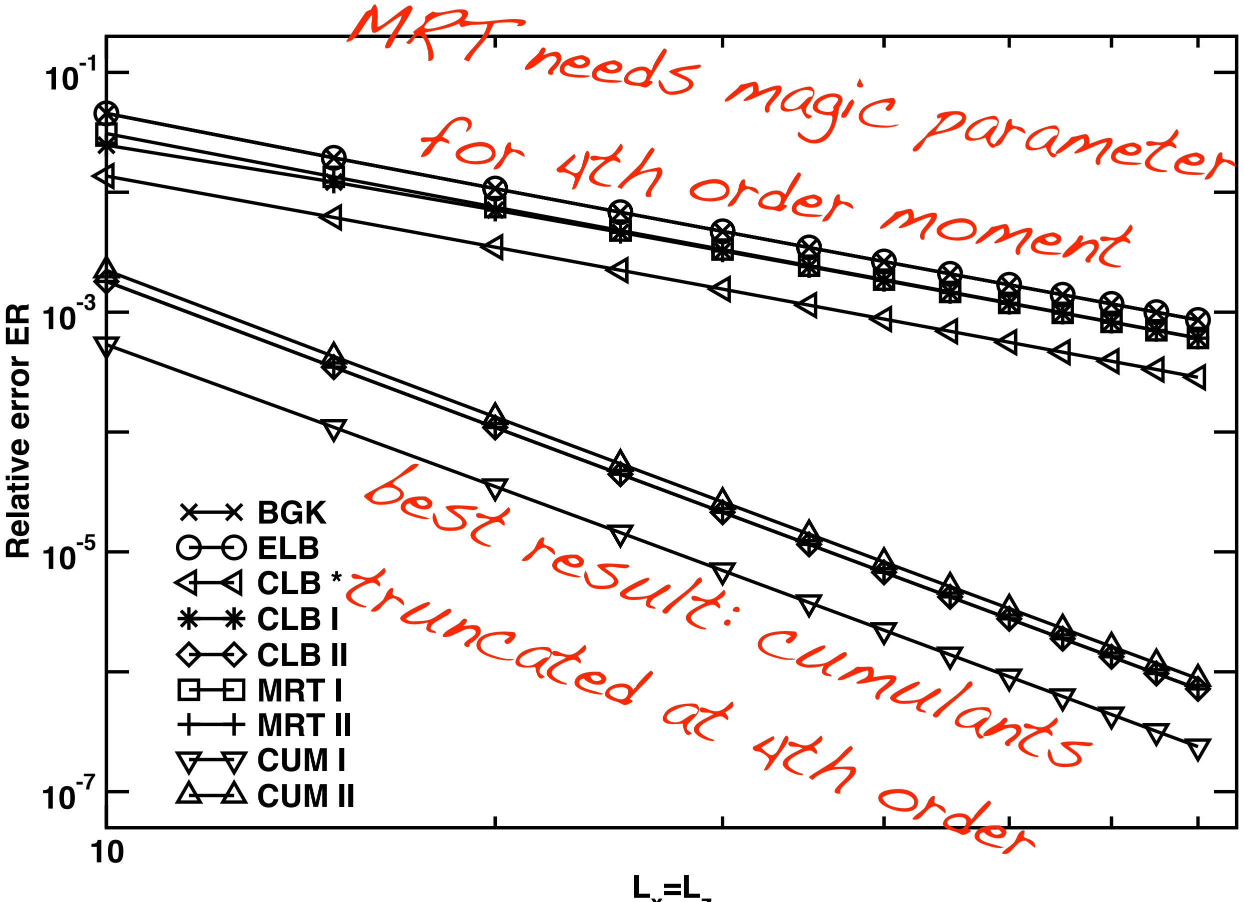
$\omega_4 : \pi_{xxy} - \pi_{yzz}$

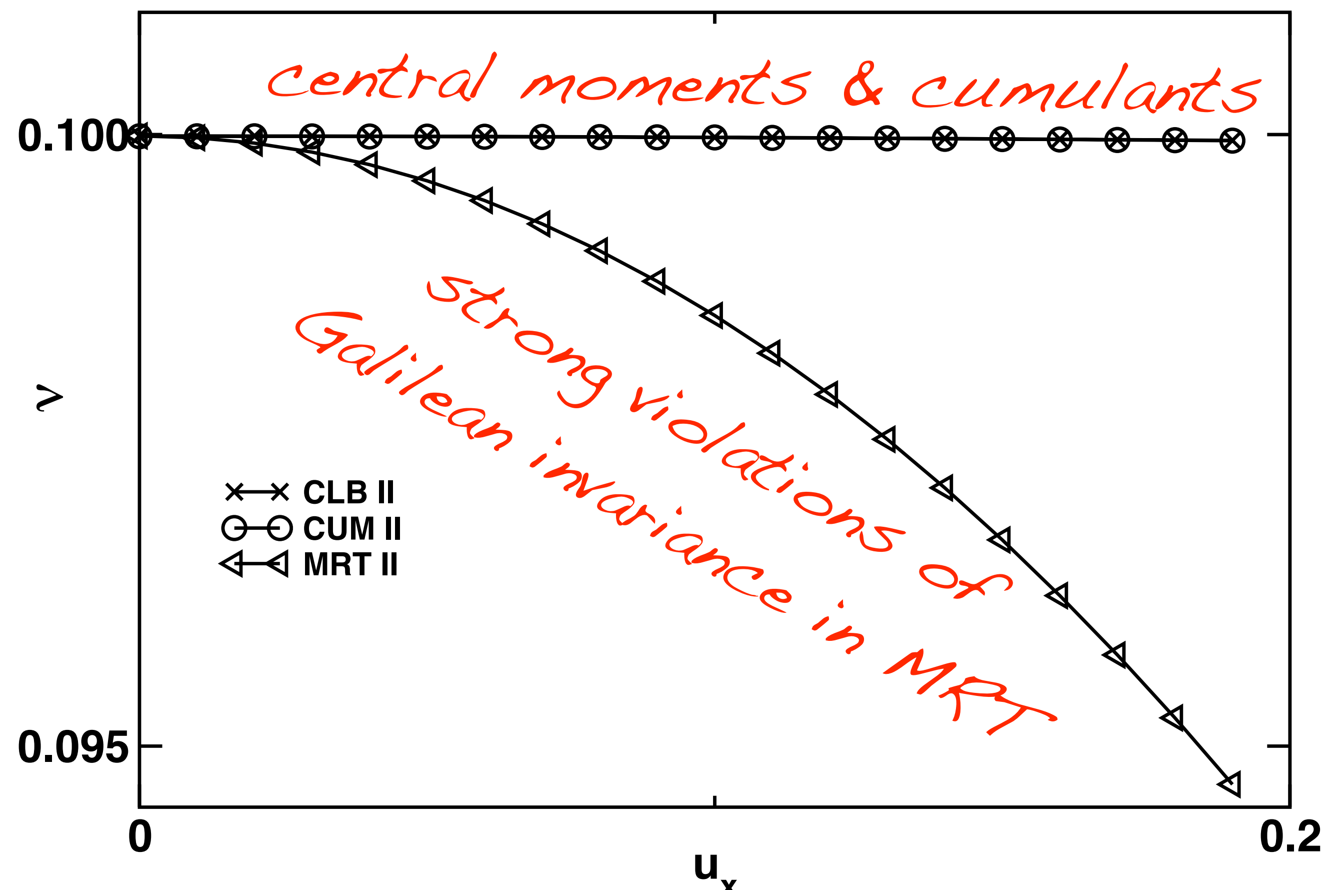
$\omega_5 : \pi_{xyz}$





Magic MRT versus magic cumulants





this makes the difference!

use cumulant equilibrium!

$O(Ma^2)$!!!

$$\pi^{at}_{xxyz} = -4\pi_y\pi_x\pi_{xz} + 2\pi_{xz}\pi_{xy} + 2\pi_x\pi_{xyz} + \pi_{yz}(\pi_{xx} - 2\pi_x^2) + \pi_y\pi_{xxz} + \pi_z(\pi_y(6\pi_x^2 - 2\pi_{xx}) + \pi_{xxy} - 4\pi_x\pi_{xy}))$$

Questionnaire

- Are parameters „magic“ or „quadric“?

Magic! I do not understand them!

- Do they help us?

If they work under general condition, then they are a big leap forward. If not, we might still learn something important from them. We have to understand them!

- Are cumulants better than moments?

Yes! Galilean invariance and stability is improved. Quadric behavior even if we equilibrate 4th cumulants. But they do not solve all problems...