Groupe de travail
“Schémas de Boltzmann sur réseau”

Institut Henri Poincaré
11 rue Pierre et Marie Curie, Paris 5 ième

Mercredi 02 novembre 2016
salle 421 (4ème étage), de 14h à 15h30

Pierre Lallemand (CNRS et CSRC, Pékin)
Anomalous Advection in LBE Simulations

Séances suivantes les
10 novembre 2016,
01 février, 01 mars, 05 avril, 03 mai, 07 juin 2017.

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ANOMALOUS ADVECTION in LBE SIMULATIONS

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- LBE Models
  - D2Q9 for diffusion
  - D2Q9 and D2Q13 for Navier-Stokes
- Mode analysis
  - Dispersion equation
  - Equivalent equations
- Errors in advection terms
- Some simulations

Diffusion with D2Q9

d'Humières approach

Moment	*Rate*	*Equilibrium*
ρ	0	ρ
j_x	s_1	ρV_x
j_y	s_1	ρV_y
E	s_3	$\rho(\alpha + 3(V_x^2 + V_y^2))$
XX	s_4	$\rho(V_x^2 - V_y^2)$
XY	s_4	$\rho(V_x V_y)$
q_x	s_6	$q\rho V_x$
q_y	s_6	$q\rho V_y$
ϖ	s_8	$\rho(\beta - 3(V_x^2 + V_y^2))$

Domain with periodic boundary conditions
Define phase factors and time increment

$$p = \exp ik_x, \quad q = \exp ik_y, \quad z$$

$$m_k(i, j, t_l) = m_{k0} p^i q^j z^l$$

with $m_1 = 1 + h\rho$, $m_2 = V_x + hj_x$ and $m_3 = V_y + hj_y$.
Linearize with respect to h.
Perform collision and propagation.

$$m_{k1} = \mathcal{Q} m_{k0} = z m_{k0}$$

Dispersion equation
State at site $\{i, j\}$

$$\Phi(i,j) = \{f_1(i,j), \cdots, f_n(i,j)\} \tag{1}$$

or moments

$$m = \mathcal{M}\Phi \tag{2}$$

One time step
Relaxation

$$m^* = (I + \mathcal{C})m \tag{3}$$

$$\mathcal{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\ s_1 V_x & -s_1 & 0 & 0 & 0 & 0 & 0 & 0 & \\ s_1 V_y & 0 & -s_1 & 0 & 0 & 0 & 0 & 0 & \\ s_3(\alpha + 3(V_x^2 + V_y^2)) & 0 & 0 & -s_3 & 0 & 0 & 0 & 0 & \\ s_4(V_x^2 - V_y^2) & 0 & 0 & 0 & -s_4 & 0 & 0 & 0 & \\ s_4 V_x V_y 0 & 0 & 0 & 0 & 0 & -s_4 & 0 & 0 & \\ s_6 q V_x & 0 & 0 & 0 & 0 & 0 & -s6 & 0 & \\ s_6 q V_y & 0 & 0 & 0 & 0 & 0 & 0 & -s_6 & \\ s_8(\beta - 3(V_x^2 + V_y^2)) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & - \end{pmatrix}$$

$$\mathcal{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha s_e & 0 & 0 & -s_e & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -s_\nu & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -s_\nu & 0 & 0 & 0 \\ 0 & -s_q & 0 & 0 & 0 & 0 & -s_q & 0 & 0 \\ 0 & 0 & -s_q & 0 & 0 & 0 & 0 & -s_q & 0 \\ \beta s_\varpi & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -s_\varpi \end{pmatrix}$$

Propagation in f space

$$\Phi_c = \mathcal{M}^{-1} m^* \tag{4}$$

Then multiply each component of Φ_c by a phase factor

$$p^{c_{ix}} \ q^{c_{iy}}$$

with

$$p = \exp ik_x, \quad q = \exp ik_y$$

to get Φ_{cp} (represented by multiplication by P_h)
For a domain with periodic boundary conditions and after linearization, one has a system of difference equations with solution

$$\Psi(t+1) = z\Psi(t) \tag{5}$$

with a time increment z given by one of the eigenvalues of the system

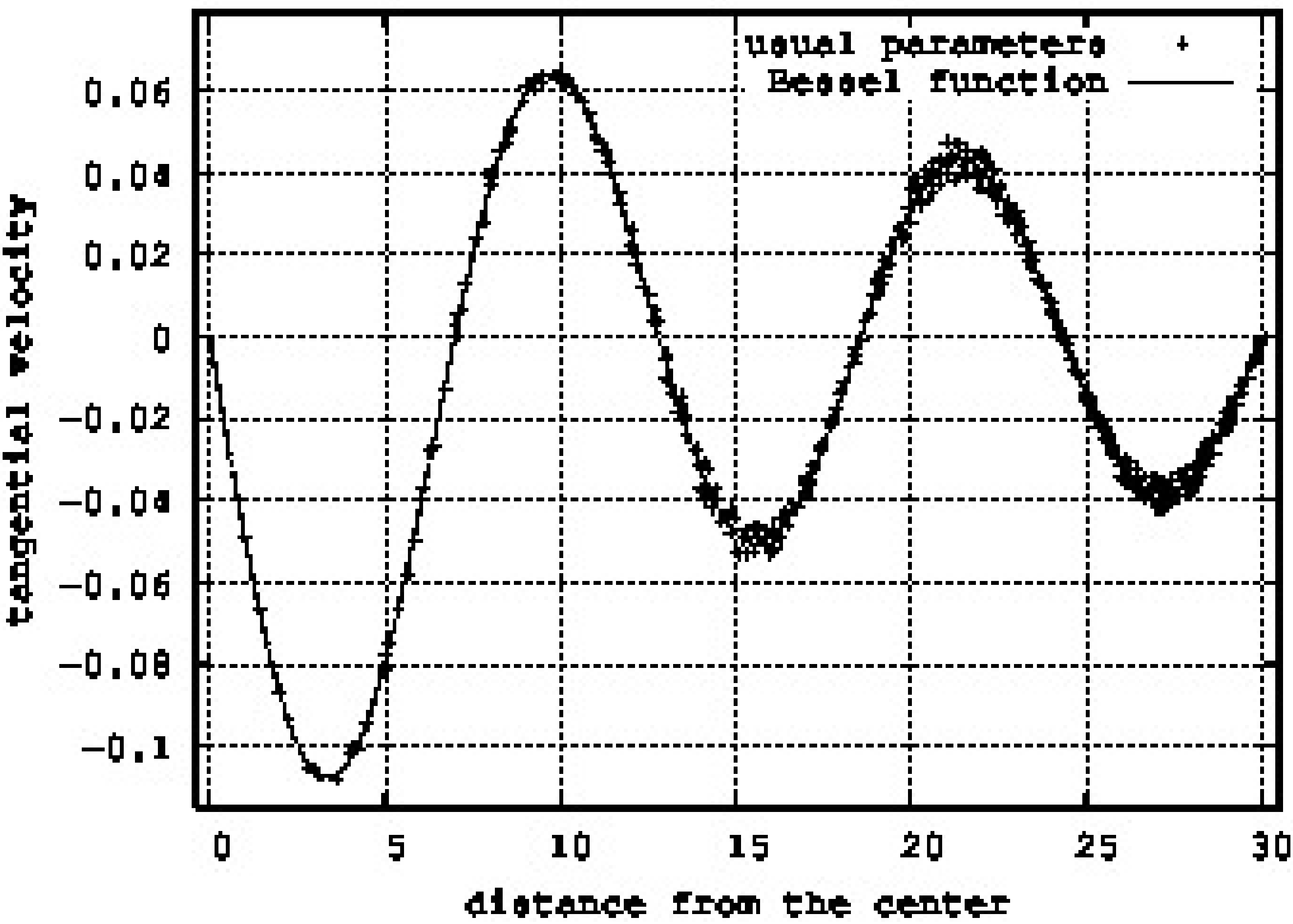
$$(\mathcal{M}^{-1}(I + \mathcal{C})\mathcal{M})P_h = zI \tag{6}$$

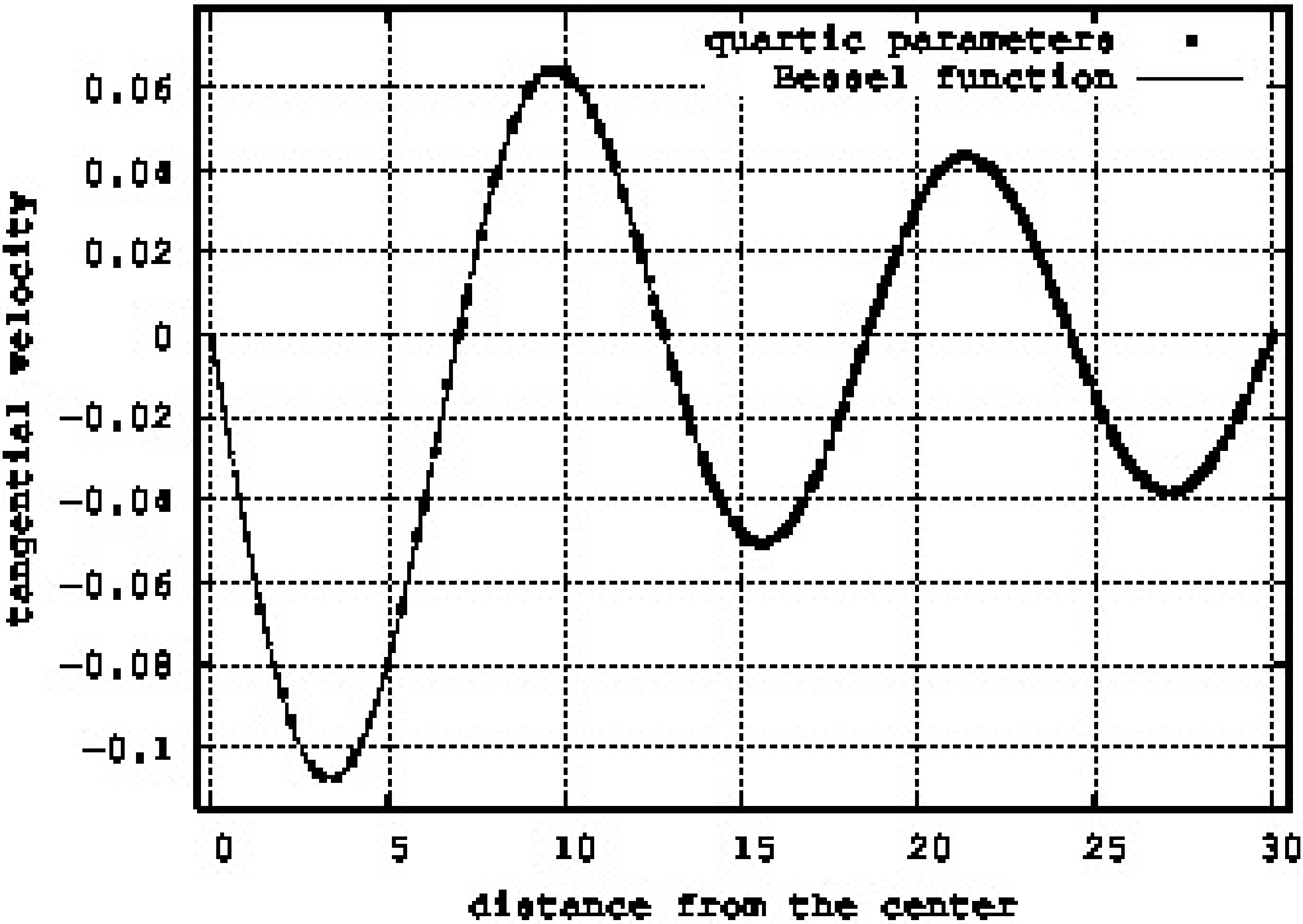
Dispersion equation is a polynomial of degree n in z.
For $k_x = k_y = 0$,

$$D(z) = (1 - z)^{n_c} \Pi_{i=n_c+1}^{n} (1 - z - s_i) \tag{7}$$

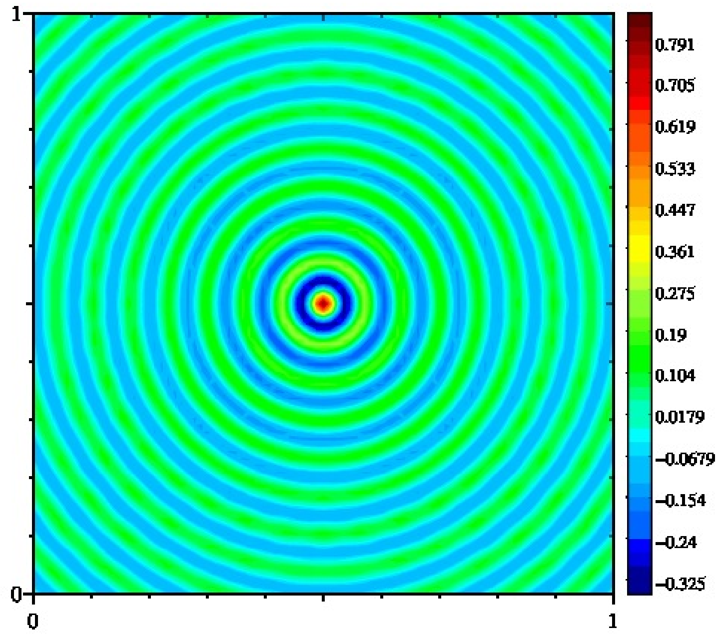
Other techniques yield $\omega(k_x, k_y)$ to be compared to $\log z$.
Although limited to periodic situations and linearized states, this is useful to determine linear stability.
For small values of $k_x,\ k_y$, hydrodynamic solutions (z close to 1), can be obtained by successive approximations.

Developments in space using space derivatives of f_s or of the moments.
For time, one can use Taylor expansion as done by Dubois, or decompose the time increment in $dt_1 + dt_2 + ..$ following Chapman-Enskog.
Up to order 2, same results.
At higher orders, the Chapman-Enskog approach is delicate due to non commutations.
So we use one of these techniques to “reduce” the 9x9 problem to a 1x1 or 3x3 system (depending on the number of conserved quantities).
One can use these reduced set of equations to compute the same quantities as with the dispersion equation.

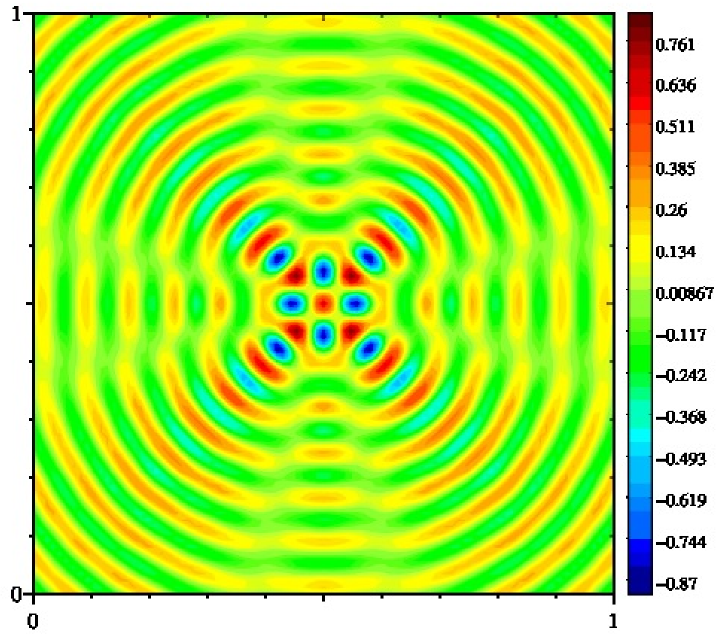

usual parameters
Bessel function
tangential velocity
0.06
0.04
0.02
0
−0.02
−0.04
−0.06
−0.08
−0.1
0
5
10
15
20
25
30
distance from the center

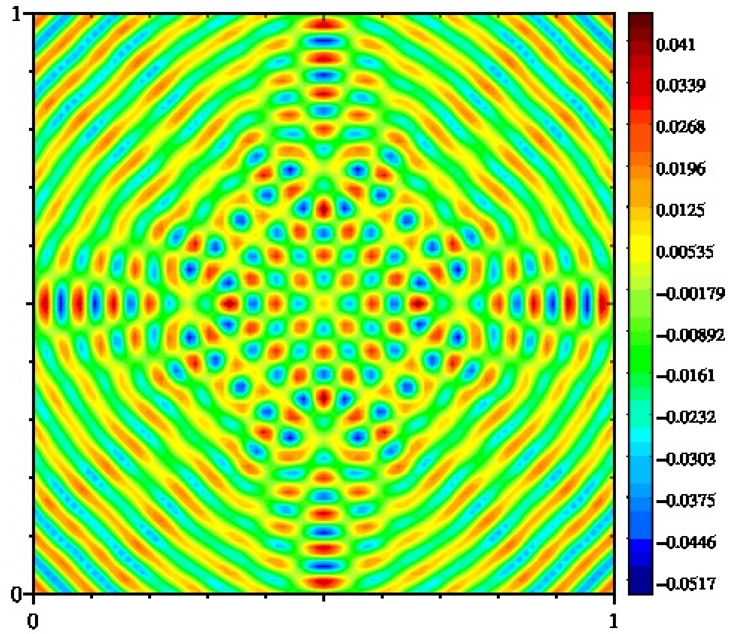


quartic parameters
Bessel function
0.06
0.04
0.02
0
−0.02
−0.04
−0.06
−0.08
−0.1
tangential velocity
0
5
10
15
20
25
30
distance from the center



1
0
0
1
0.791
0.705
0.619
0.533
0.447
0.361
0.275
0.19
0.104
0.0179
−0.0679
−0.154
−0.24
−0.325


1
0
0
1
0.761
0.636
0.511
0.385
0.26
0.134
0.00867
-0.117
-0.242
-0.368
-0.493
-0.619
-0.744
-0.87



1
0
0
1
0.041
0.0339
0.0268
0.0196
0.0125
0.00535
−0.00179
−0.00892
−0.0161
−0.0232
−0.0303
−0.0375
−0.0446
−0.0517

Properties of D2Q9 for diffusion
- Usual Chapman-Enskog treatment $\leadsto$ diffusivity κ

$$\kappa = \frac{\alpha + 4}{6}(\frac{1}{s_1} - \frac{1}{2})$$

independent of $V_x,\ V_y$.
- Equivalent equations

$$\partial_t \rho + V_x \partial_x \rho + V_y \partial_y \rho + \kappa \Delta \rho + \mathcal{O}_3 = 0$$

with

$$\mathcal{O}_3 = \sum_{abc} H_{abc}(V_x, V_y) \partial_{abc} \rho$$

odd terms contribute to the phase and thus modify advection.

For plane wave of wave vector $\{k_x,\ k_y\}$, phase factor

$$\frac{V_x k_x + V_y k_y}{k}(1 + A(k_x, k_y))$$

A of order 2 in k.
Isotropy is obtained for

$$q = -1 \quad \text{or} \quad \sigma_1\sigma_4 = \frac{1}{12}$$

$\sigma_i = \frac{1}{s_i} - \frac{1}{2}$ (Hénon parameter)
for $q = -1$

$$A_0 = \frac{1}{24}(2 + \alpha + \sigma_1(4\alpha\sigma_3 - 8\sigma_4) + \sigma_1^2(32 + 8\alpha))$$

for $\sigma_1\sigma_4 = \frac{1}{12}$

$$A_0 = \frac{1}{72}(7 - q + 3\alpha + 12\sigma_1\sigma_3(1 - \alpha + q) - \sigma_1^2(96 + 24\alpha))$$

Next order in the development in equivalent equations leads to corrections to the diffusivity.

$$\kappa(k) = \kappa_0(1 + \kappa_2 f(k))$$

where $f(k)$ is second order in k. κ_2 is the "hyperdiffusivity". It has been discussed, among others, at DFSD in Florianopolis (august 2008).

Athermal fluid simulated with D2Q9

The model is very similar to the thermal case, however there are 3 conserved moments and thus 3 equivalent equations.

Moment	*Rate*	*Equilibrium*
ρ	0	ρ
j_x	0	j_x
j_y	0	j_y
E	s_3	$\rho\alpha + 3(j_x^2 + j_y^2)/\rho$
XX	s_4	$(j_x^2 - j_y^2)/\rho$
XY	s_4	$(j_x j_y)/\rho$
q_x	s_6	$-j_x$
q_y	s_6	$-j_y$
ϖ	s_8	$\rho\beta - 3(j_x^2 + j_y^2)/\rho$

Consider a small amplitude flow (ρ, j_x, j_y) carried by a large velocity field V_x, V_y. The equivalent equation split in space derivatives of increasing order can be put as

$$M_0 = \begin{pmatrix} \partial_t & 0 & 0 \\ 0 & \partial_t & 0 \\ 0 & 0 & \partial_t \end{pmatrix}$$

$$M_1 = \begin{pmatrix} 0 & \partial_x & \partial_y \\ (\frac{\alpha+4}{6} - V_x^2)\partial_x - V_x V_y \partial_y & 2V_x\partial_x + V_y\partial_y & V_x\partial_y \\ (\frac{\alpha+4}{6} - V_y^2)\partial_y - V_x V_y \partial_x & V_y\partial_x & V_x\partial_x + 2V_y\partial_y \end{pmatrix}$$

Cumbersome expressions for M_2, M_3, etc...

Case of plane waves :

$$\begin{aligned} D(x,y,t) &= 1+\rho(0)\exp(\omega t)\cos(k_x x+k_y y) \\ J_x(x,y,t) &= V_x + j_x(0)\exp(\omega t)\cos(k_x x+k_y y) \\ J_y(x,y,t) &= V_y + j_y(0)\exp(\omega t)\cos(k_x x+k_y y) \end{aligned} \quad (8)$$

Apply a rotation of angle θ to put the Ox axis along the wave vector to highlight the presence of 2 longitudinal modes (sound modes) and 1 transverse mode (shear mode).
For an applied velocity V perpendicular to the wave vector,

$$M_0 + M_1 = \begin{pmatrix} \omega & k & 0 \\ \frac{\alpha+4}{6}k & \omega & 0 \\ 0 & V\ k & \omega \end{pmatrix}$$

$$M_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{\alpha\sigma_3-2\sigma_4}{6}(1-3V^2)k^2 & 0 \\ \frac{\alpha+4}{6}V\sigma_4 k^2 & 0 & -\frac{1}{3}\sigma_4 k^2 \end{pmatrix}$$

At order 3,

$$M_3 = \begin{pmatrix} 0 & -\frac{1}{18} & 0 \\ h_0 + h_1 V^2 & g_1 f_1(\theta) & h_3 V - g_3 V f_2(\theta) \\ g_2 V^2 f_1(\theta) & h_4 V - g_2 V^2 f_1(\theta) & g_2 V f_1(\theta) \end{pmatrix} k^3$$

with coefficients h_i and g_i depending on the relaxation rates and $f_1(\theta) = \sin 4\theta$ and $f_2(\theta) = \sin^2 2\theta$.
For $\alpha = -2$ and $\beta = 1$ (standard values for D2Q9), the angular dependences in M_3 are eliminated when $\sigma_3 = \sigma_4$ and $\sigma_4 \sigma_6 = 1/12$.

Summary

-Shear wave for V perppendicular to k

Order	Phase Velocity	Damping
1	0	
2		$\sigma_4/3$
3	$V(1-12\sigma_4\sigma_6)f_1(\theta)/24$	

-Shear wave for V parallel to k

Order	Phase Velocity	Damping
1	V	
2		$\sigma_4/3(1-3V^2)$
3	$V(\frac{2\sigma_4(\sigma_4-\sigma_6)}{3}+\frac{1-12\sigma_4\sigma_6}{24}f_2(\theta))$	

Similar expressions are readily obtained for acoustic waves showing dissymmetries between forward and backward propagating sound waves.

Athermal fluid simulated with D2Q13
The main difference with D2Q9 occurs in the presence of 2 additional heat flux moments allowing to eliminate the velocity dependence of the shear viscosity.
Partial table of moments

Moment	*Rate*	*Equilibrium*
q_x	s_6	$j_x(c1 - \frac{36q-35}{77}(j_x^2 + j_y^2))$
q_y	s_6	$j_y(c1 - \frac{36q-35}{77}(j_x^2 + j_y^2))$
r_x	s_8	$j_x(-\frac{63c_1+65}{24} + qj_x^2 + \frac{42q-105}{22}j_y^2)$
r_y	s_8	$j_y(-\frac{63c_1+65}{24} + qj_y^2 + \frac{42q-105}{22}j_x^2)$

Summary

-Shear wave and V perpendicular to k

Order	Phase Velocity	Damping
1	0	
2		$\frac{3+c_1}{4}\sigma_4(1-\frac{21}{77}\frac{7+6q}{3+c_1}V^2)$
3	$\frac{\sigma_4(89772\sigma_6+30888\sigma_8)-10055}{157080}Vf_1(\theta)$	

-Shear wave and V parallel to k

Order	Phase Velocity	Damping
1	V	
2		$\frac{3+c_1}{4}\sigma_4(1-\frac{21}{77}\frac{7+6q}{3+c_1}V^2)$
3	$V(C+Df_2(\theta))$	

with an angular dependence (D) that can be suppressed for :

$$\sigma_6=\sigma_8=\frac{1}{12\sigma_4}$$

for which the constant term (C) is :

$$C=\frac{3+c_1}{24}(12\sigma_4^2-1)$$

Example of anomalous advection
V along X-axis, k (of modulus 1) at an angle θ.

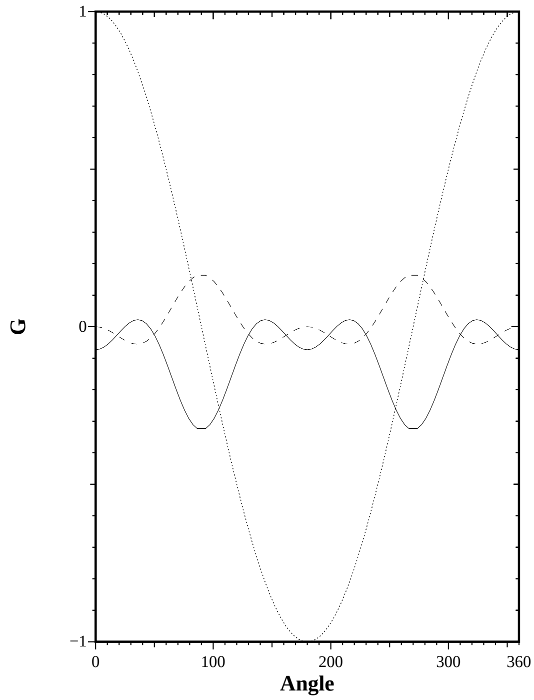


Figure : D2Q13 : solid line, D2Q9 : dashed line.

Test on Plane Waves with D2Q13
Domain : square 240×240
with periodic boundary conditions.
Initial conditions :

$$
\begin{aligned}
D(x, y, 0) &= 1 + \rho_0 \ \cos k_x x + k_y y \\
J_x(x, y, 0) &= V_x + j_{x0} f_x(x, y) \\
J_y(x, y, 0) &= V_y + j_{y0} f_y(x, y)
\end{aligned}
$$

f_x and f_y (appropriate sum of cos and sin).
During simulation, measure correlation functions, $C_\rho(t)$, $C_x(t)$, $C_y(t)$.

Relaxation of shear waves

Two groups of 4 cases are simulated for the same set of wave vector :

	k_x/k_0	k_y/k_0	k/k_0
A	5	12	13
B	10	24	26
C	13	0	13
D	26	0	26

with $k_0 = \frac{2\pi}{240}$.
In both cases there is a uniform velocity $V = 0.07$ which is either perpendicular or parallel to the wavec vector.

Shear Wave for V perpendicular to K

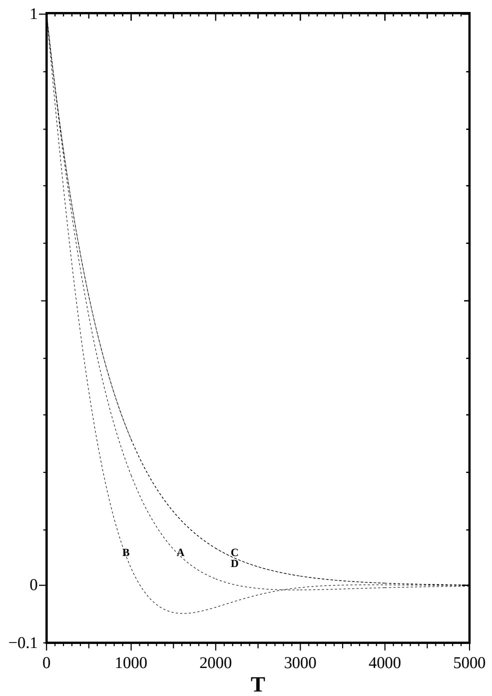


Figure : Relaxation of shear waves. Uniform velocity perpendicular to the wave vector.

Case V parallel to K

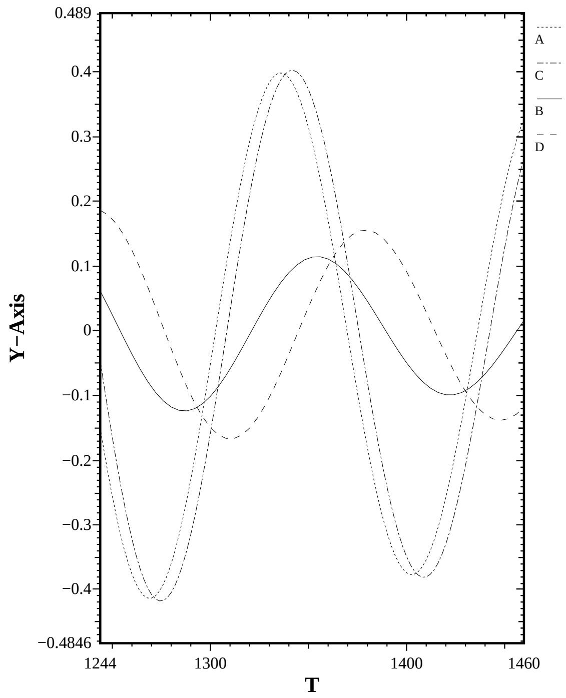


Figure : Shear wave for a uniform velocity parallel to the wave vector.

For the parallel case, the phase velocity is given in units of the exact value $k\ V$.

Case	Theory	Measurement
A	0.9960	0.9959
B	0.9840	0.9827
C	0.9917	0.9915
D	0.9666	0.9652

Gaussian initial conditions

$$\rho(r,0) = g_0 \exp -(\frac{r}{r_0})^2$$

at time t

$$\rho(r,t) = g_0 \frac{r_0^2}{r_0^2 + 4\kappa t} \exp - \frac{(x - V_x t)^2 + (y - V_y t)^2}{r_0^2 + 4\kappa t}$$

Same formulae for the stream function (κ replaced by ν).

D2Q9 for diffusion

Periodic domain 101^2. $r_0 = 5.0, \kappa = 0.008, V_x = 0.10, V_y = 0.00$, 3200 time steps.

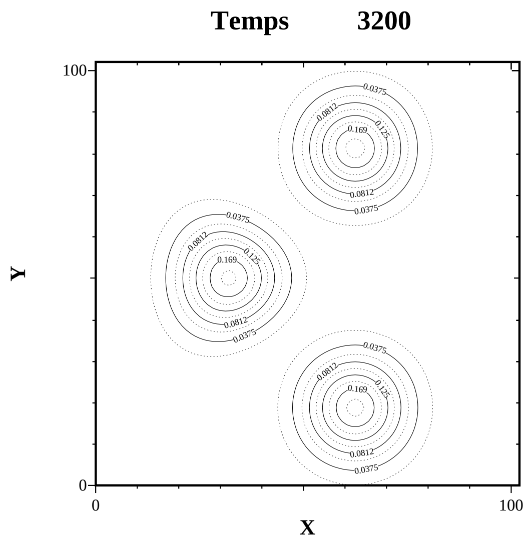
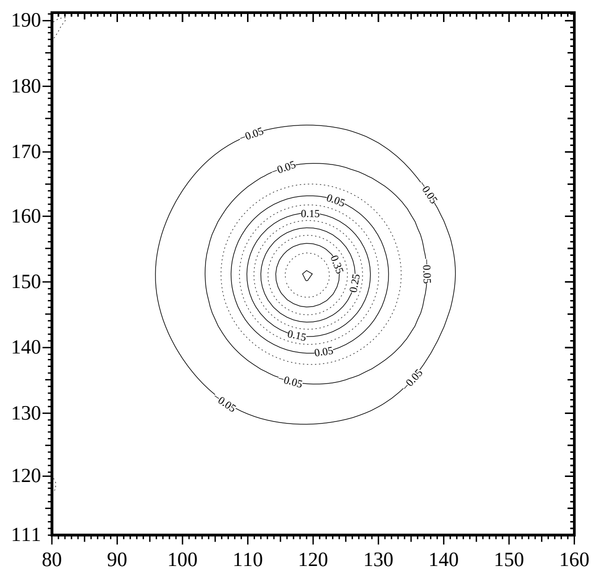
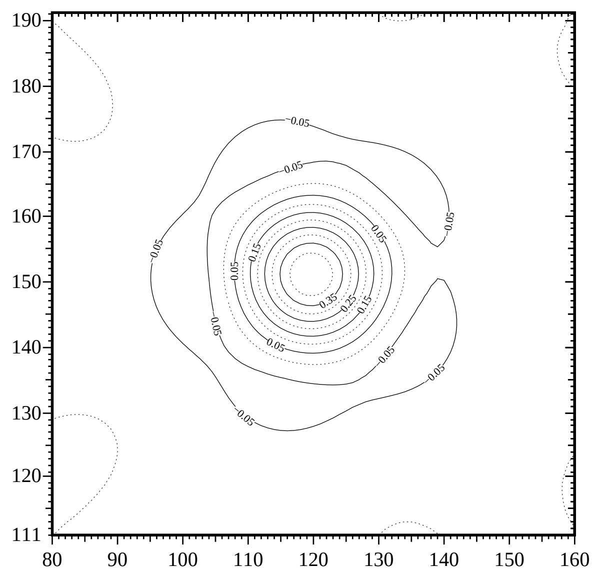


Figure : Middle : any parameters. Top :$q = -1$. Bottom : $12\sigma_1\sigma_4 = 1$.

D2Q9 for flow

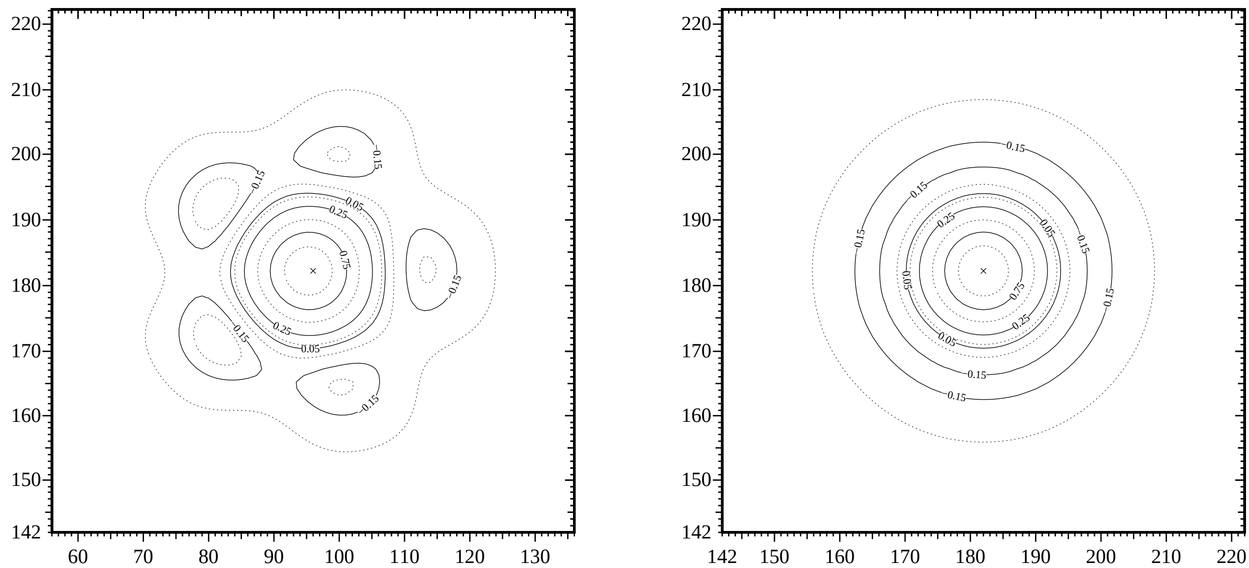
$r0 = 8.0$, $\nu = 0.0035$ $V_x = .03$, 9000 time steps. Left : $12\sigma_4\sigma_6 = 1$.





D2Q13 for flow

$r_0 = 11.0$, $\nu = 0.003$, 2770 time steps. $V_x = .10$ at left, 0 at right.



Introduction of anomalous advection in a spectral code.
The initial state of the gaussian dot situated in a square periodic domain can be written in Fourier Transform space as

$$\pi r_0^2 \sum_{k_x, k_y} \exp(-r_0^2 (k_x^2 + k_y^2)/4)$$

In a linear regime, each Fourier component evolves as

$$\exp(-\nu(k_x^2 + k_y^2) + Ig(k)V)t$$

A backward Fourier transformation can then be performed.
Domain size 80^2 (use Temperton FFT), initial $r_0 = 4.0$, Main velocity at 14° from Ox. $g(k) = 1 + 0.01(\cos 4\theta - \cos 2\theta)k^2$.

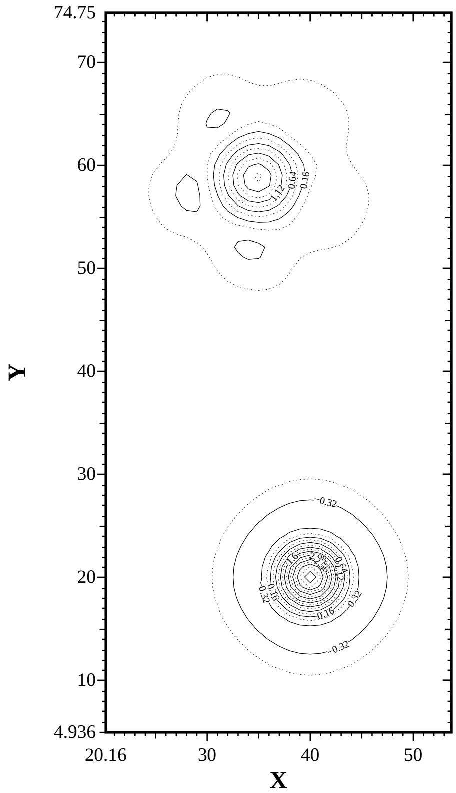


Figure : Top : after travelling twice the size of the domain , Bottom, initial state.

Unsolved question

How to analyze non linear situations even in the simpler case where the advective part is a plane wave ?

Early work was done for the Taylor-Green vortex with d'Humières.

It was observed that successive spatial harmonics of D3Q13 (and D3Q19) did not appear in time as computed with an accurate spectral code.

Case : square periodic domain 144×144 for LBE and 72×72 for spectral case, with periodic boundary conditions.

Initial conditions : sum of two plane waves

$k_1 = \{2, 1\}$, amplitude a_1

$k_2 = \{5, 4\}$, amplitude a_2

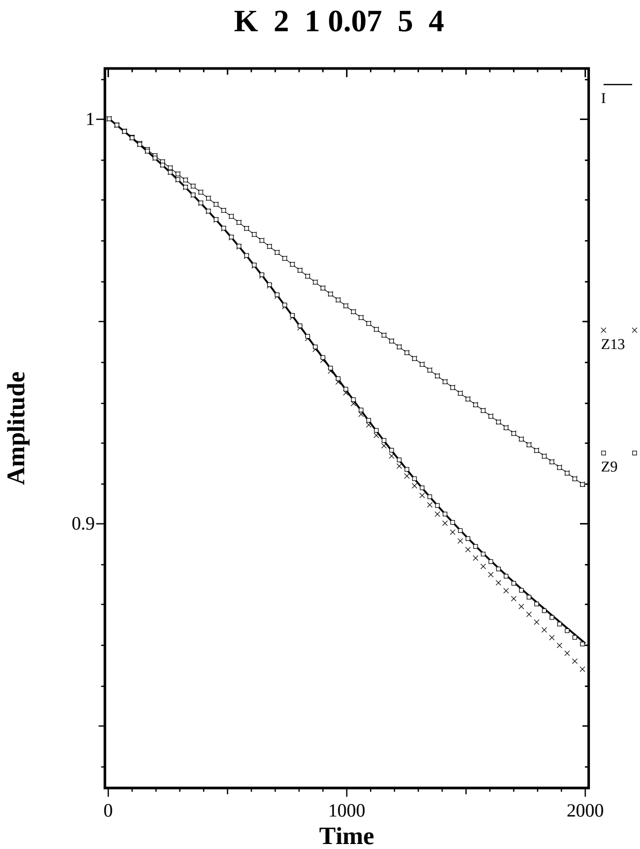


Figure : Relaxation of the initial waves.

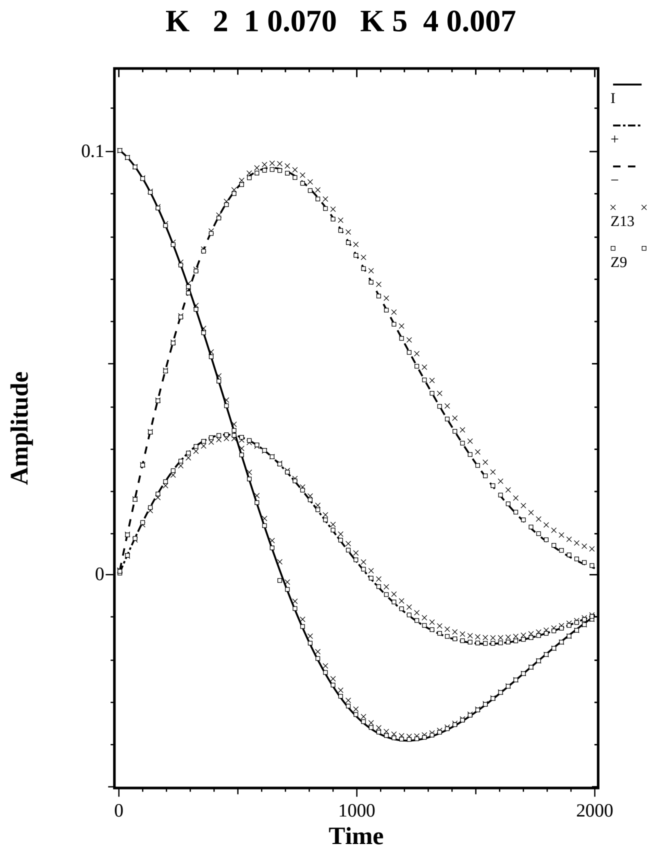


Figure : Relaxation of the initial wave and generation of the first "beat-notes"

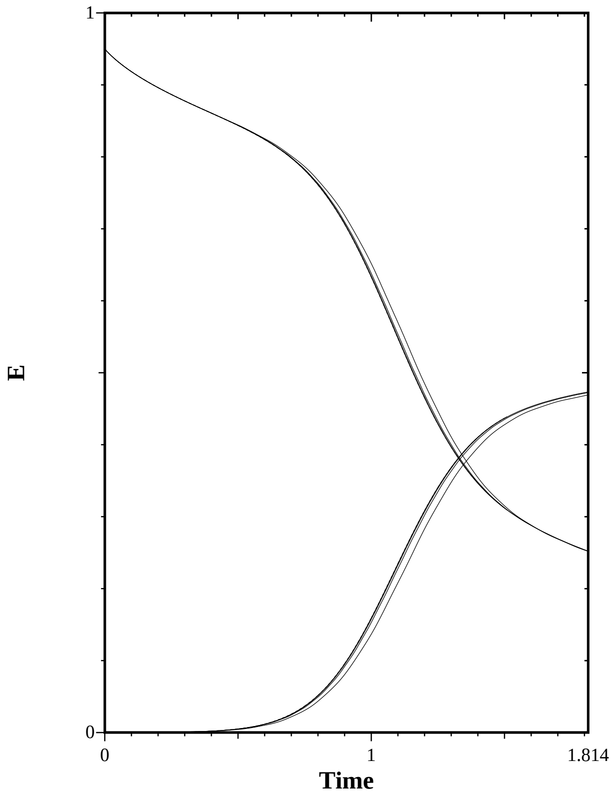


Figure : Minion situation. Time evolution of v_x^2 and v_y^2 computed with D2Q9, D2Q13 and Spectral-FFT.

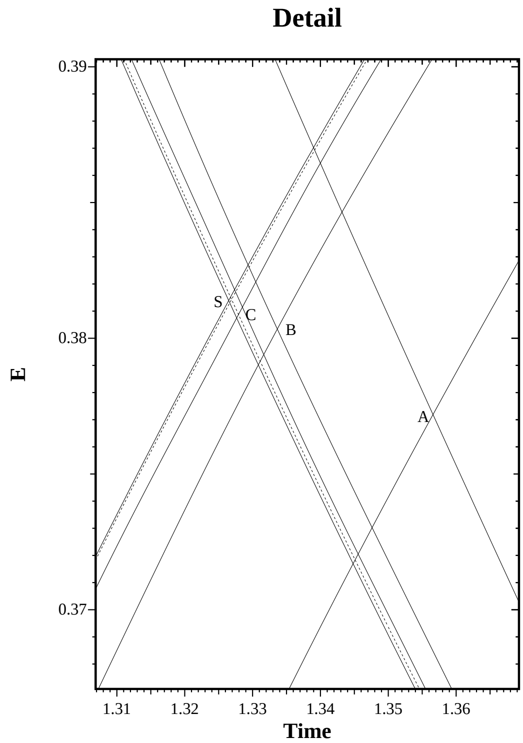


Figure : Minion situation. Detail of the time evolution of v_x^2 and v_y^2 computed with D2Q9, D2Q13 and Spectral-FFT. {A, B, C}, (0.10, 0.05, 0.025). S spectral, dashed line D2Q13.

3-d Taylor-Green
Mode 4,6,4