Extended BGK-Boltzmann equation with *H*-Theorem for dense gases

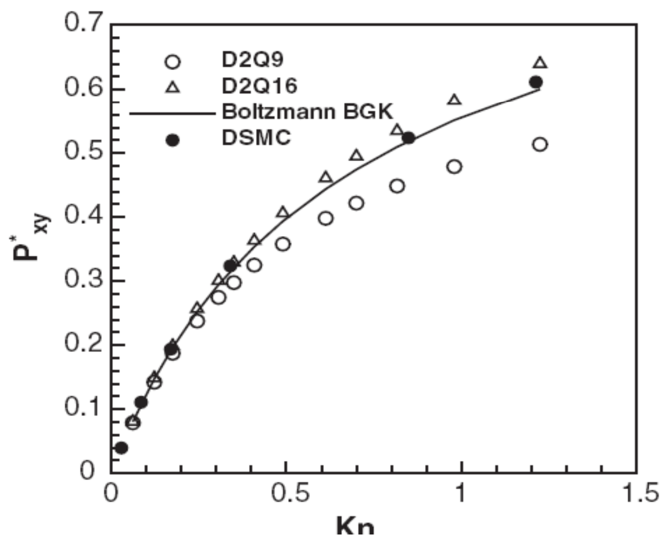
Saikishan Suryanarayanan
Shiwani Singh
Santosh Ansumali

JNCASR , Bangalore

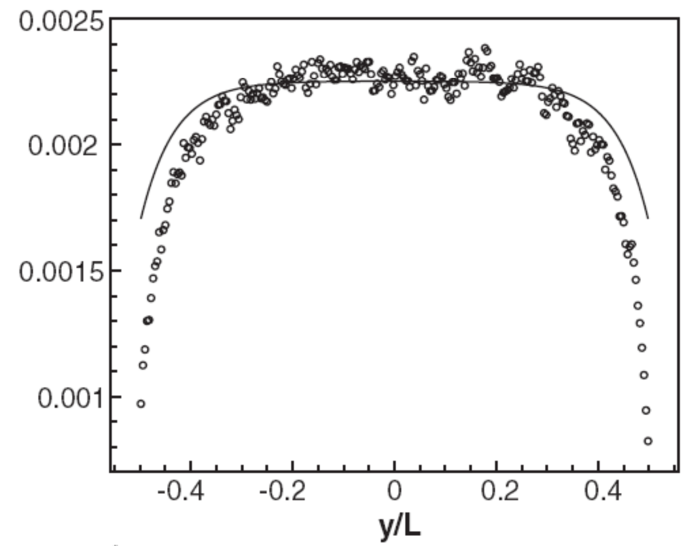
Lattice Boltzmann Methods for Dilute Gases

- The Bhatnagar-Gross-Krook (BGK) collision model -
  Physically intuitive and easy to implement.

- With appropriate boundary conditions,
  the **LBM with BGK is a good model for studying dilute gases** even at molecular regime.



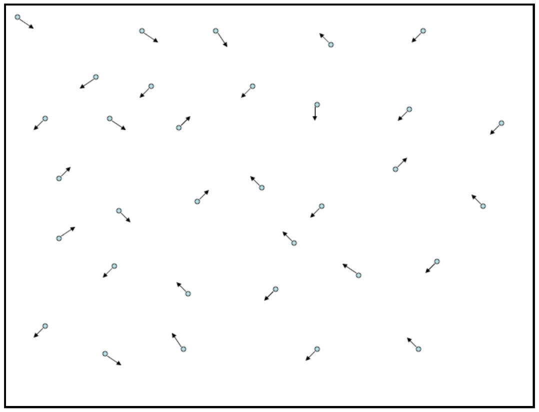
Shear stress at various Knudsen numbers.
$P^*_{xy} = P_{xy}/$ shear stress at Kn $\rightarrow \infty$ of Boltzmann-BGK

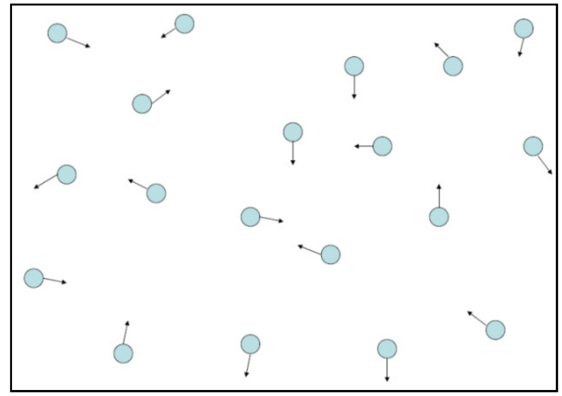


Nonequilibrium normal stress difference at Kn $= 0.6$. symbol: DSMC simulation.

Ref: Ansumali et al, *Phys Rev Lett,* 98, 124502 (2007)

Extension to Dense Gases





- In dense gases, the **collision is no longer local**.
- Boltzmann equation was extended by Enskog for dense gases by accounting for non-ideal effects in collision term.

$$J = a^2 \int_{\mathcal{R}^3} \int_{B-} d\mathbf{w} d\mathbf{n} \Big[g_2(\mathbf{x}, \mathbf{x} - a\mathbf{n})\, f(\mathbf{x}, \mathbf{v}') f(\mathbf{x} - a\mathbf{n}, \mathbf{w}')$$
$$- g_2(\mathbf{x}, \mathbf{x} + a\,\mathbf{n}) f(\mathbf{x}, \mathbf{v}) f(\mathbf{x} + a\,\mathbf{n}, \mathbf{w}) \Big] |(\mathbf{w} - \mathbf{v}) \cdot \mathbf{n}|,$$

- *H* – Theorem exists. *H* function defined as $H(\mathbf{x},t) = H^{\mathrm{id}} - \dfrac{s^{\mathrm{nid}}(\rho(\mathbf{x},t))}{R}.$

- It is very difficult to solve Enskog equation analytically or numerically.

  Is there a phenomenological model like BGK for dense gases ?

Issues in extending BGK for dense gases

1. Equilibrium distribution is still of Maxwell-Boltzmann form but non-ideal contribution to pressure – BGK cannot be directly used !

$$\partial_t j_\gamma + \partial_\alpha \left[\rho u_\alpha u_\gamma + \rho T \, \delta_{\alpha\gamma} + \sigma_{\alpha\gamma} \right] = -\partial_\gamma p^{nid}$$

2. Equilibrium entropy is that of a non-ideal gas.
3. A part of collision term should contribute to the entropy flux rather than entropy production.

Prior attempts to extend BGK for dense gases

Involve expanding Enskog integral around the BGK collision term.

$$J = \frac{1}{\tau}\left(f^{\mathrm{MB}} - f\right) + \sum f^{\mathrm{MB}}\mathbf{C}^{(n)}\,\mathbf{H}^{(n)}(\boldsymbol{\xi})$$

Where $\boldsymbol{C}^{(n)}$ is tuned to get correct conservation laws

Ref: Dufty et al, *Phys. Rev. Lett.* 77 1270, (1996)
Lutsko et al, *Phys. Rev. Lett.* 78 243, (1997)
Luo L.S., *Phys. Rev. Lett.* 81 1618, (1998)

Unresolved Issues

1. No *H*- Theorem for this formulation.
2. Incorrect thermal conductivity behavior.

Note :

Most existisng multiphase LB models are of this class. Further, density dependence of viscosity is not accounted in many such studies

Present Model

- In the present model, the non ideal effects are accounted by **modification of the advection term.**
  (Motivation : Effect of collective motion on the tagged particles during the mean free time.)

$$\partial_t f(\mathbf{z},t) + \partial_\alpha \left[f(\mathbf{z},t)\, \hat{\mathrm{v}} \right] = \mathcal{J}$$

- The propagation velocity is written as a formal Hermite expansion and most general form consistent with the conservation laws, is

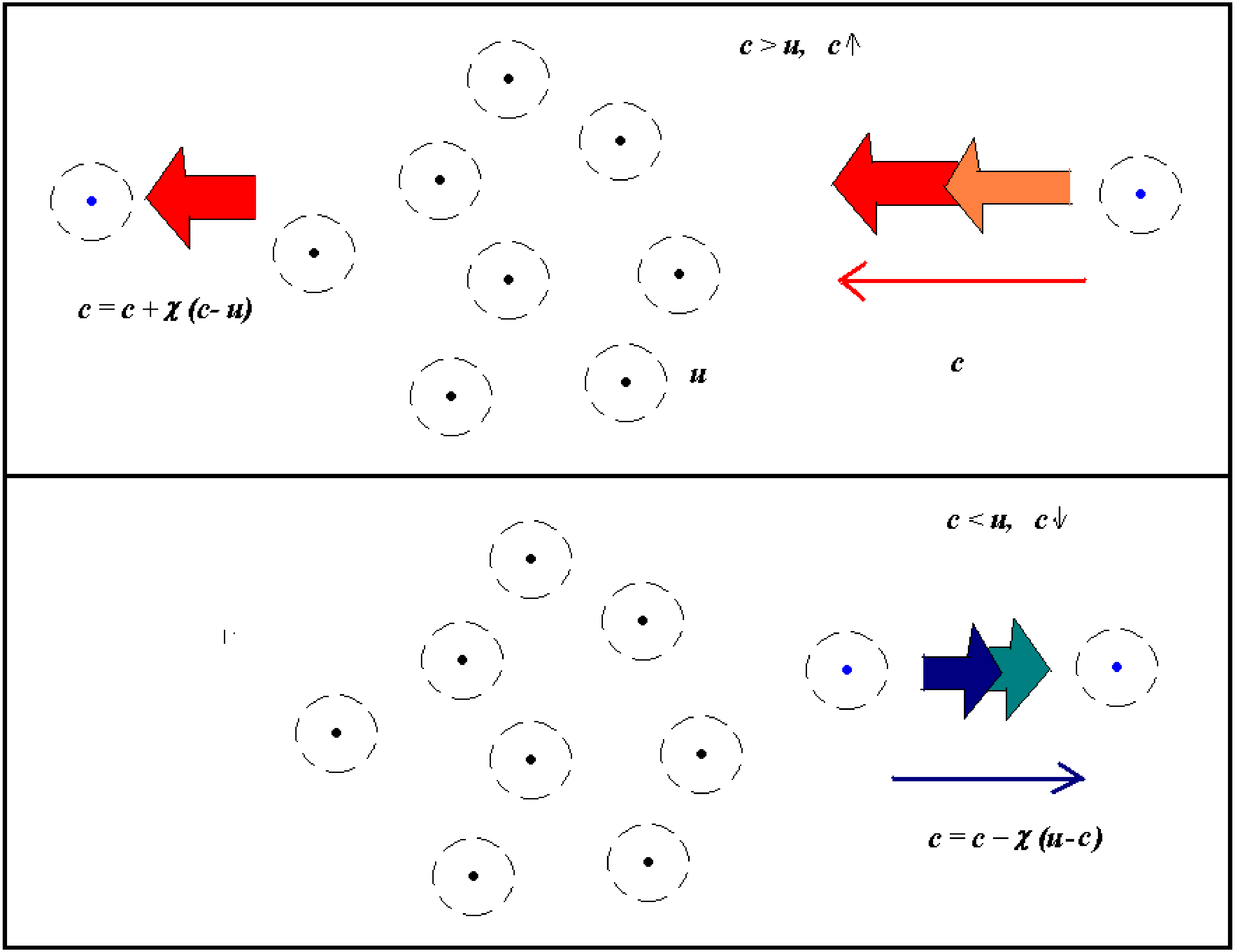
$$\hat{v}_\alpha - c_\alpha = \underbrace{\chi\left(c_\alpha - u_\alpha\right)}_{A} + \underbrace{\left(c_\beta - u_\beta\right)\frac{P^{(1)}_{\alpha\beta}}{\rho R T}}_{B} + \underbrace{u^{(1)}_\alpha\left(\xi^2 - \frac{D}{2}\right)}_{C}$$

Used in present study

Used for independently setting transport coefficients.
Not considered in present simulations

Where $$\chi = \frac{p}{\rho R T} - 1 \equiv \frac{1}{\rho R}\left(s^{\mathrm{nid}} - \rho\frac{\partial s^{\mathrm{nid}}}{\partial \rho}\right)$$

Ref : Ansumali, *Commun. Comput. Phys., 9 ,pp. 1106-1116, (2011)*



$c > u, \quad c\uparrow$
$c = c + \chi\,(c- u)$
u
c
$c < u, \quad c\downarrow$
$c = c - \chi\,(u-c)$

H - Theorem

$$H(\mathbf{x},t) = H^{\mathrm{id}} - \frac{s^{\mathrm{nid}}(\rho(\mathbf{x},t))}{R}.$$

where $H^{\mathrm{id}}(\mathbf{x},t) = \int d\mathbf{v}\, f(\mathbf{x},\mathbf{v},t)\,[\log f(\mathbf{x},\mathbf{v},t) - 1]$

$$\partial_t H + \partial_\alpha J_\alpha^{\mathrm{H}} = \int \mathcal{J} \log f\, d\mathbf{v}.$$

with the flux of H-function (analog of entropy flux) is

$$J_\alpha^{\mathrm{H}} = -\left(\frac{s^{\mathrm{nid}}}{R} u_\alpha\right) + \int d\mathbf{v}\,[f(\log f - 1)\,\hat{v}_\alpha]$$

H-theorem is valid if entropy production is positive, i.e. right side must be negative.

It is always satisfied for Boltzmann or BGK as $\int \mathcal{J} \log f\, d\mathbf{v}$ is negative.

Ref : Ansumali, *Commun. Comput. Phys., 9 ,pp. 1106-1116, (2011)*

Conservation Equations

- On talking moments, the present model leads to the following mass and momentum conservation equations

$$\partial_t \rho + \partial_\alpha j_\alpha = 0$$
$$\partial_t j_\gamma + \partial_\alpha \left[\rho u_\alpha u_\gamma + p\delta_{\alpha\gamma} + \sigma_{\alpha\gamma}\right] = 0$$
$$\partial_t E + \partial_\alpha \left[(E+p) u_\alpha + \sigma_{\alpha\gamma} u_\gamma + q_\alpha\right] = 0$$

upto first order in *Kn* ,

$$\sigma_{\alpha\beta} = -\eta \left(\partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{D}\partial_\gamma u_\gamma \delta_{\alpha\beta}\right)$$
$$q_\alpha = -\tau \left\{ p\,(1+\chi^h)\, C_p \right\} \partial_\alpha T$$

Ref : Ansumali, *Commun. Comput. Phys., 9 ,pp. 1106-1116. (2011)*

DSMC for dense gases

- Stochastic technique, much cheaper than MD.
- Two steps : Advection (particles move with const. velocity) & Collision.
- Randomly selected particles are chosen as candidates for collision.
- The pair is selected if condition on relative velocity is satisfied
- Post- collision velocities are determined stochastically based on kinetic theory.

ALDER'S ALGORITHM FOR DENSE GASES

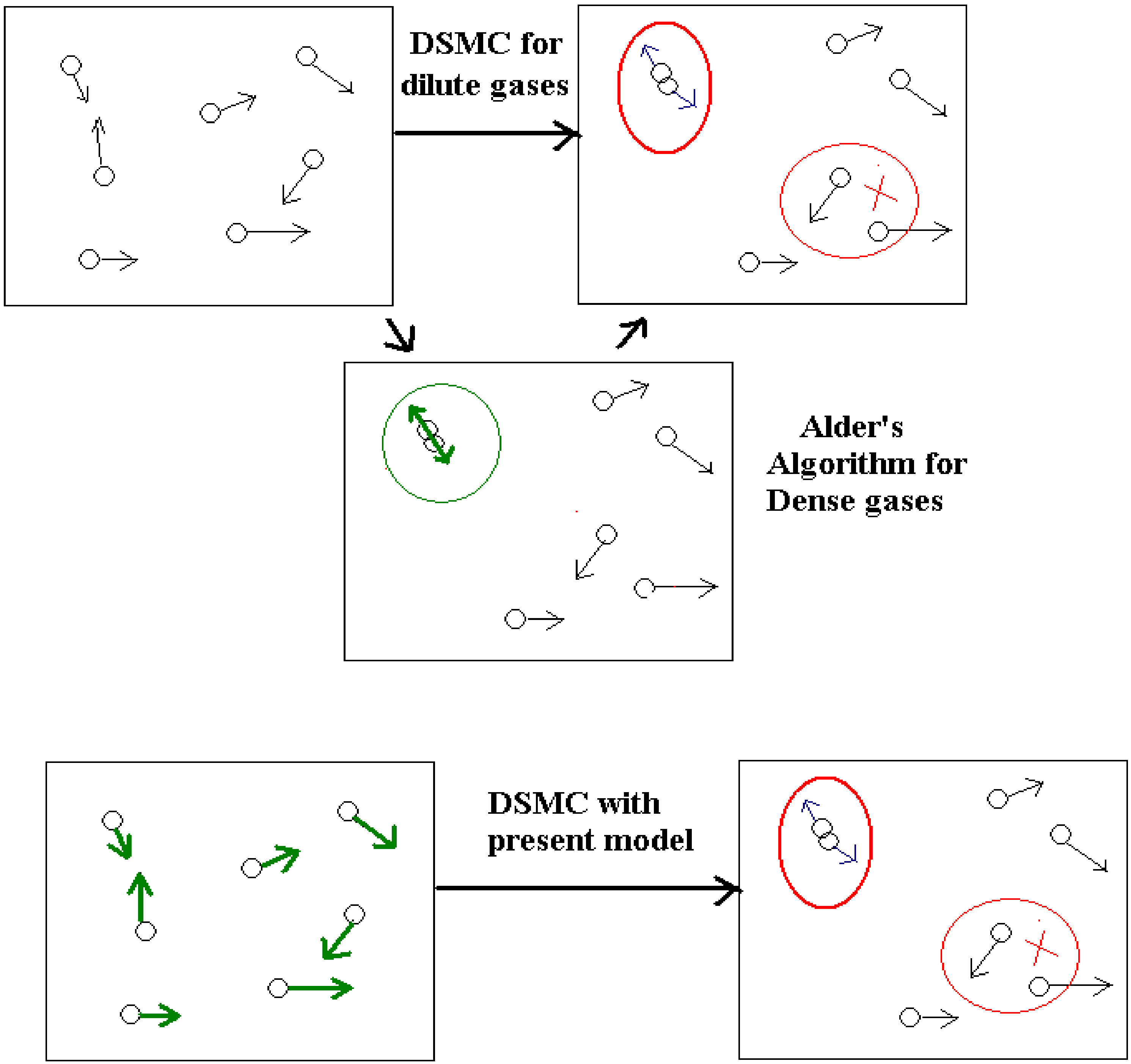
- Accounts for size of particle by displacing particles that are within particle size.

DSMC OF PRESENT MODEL

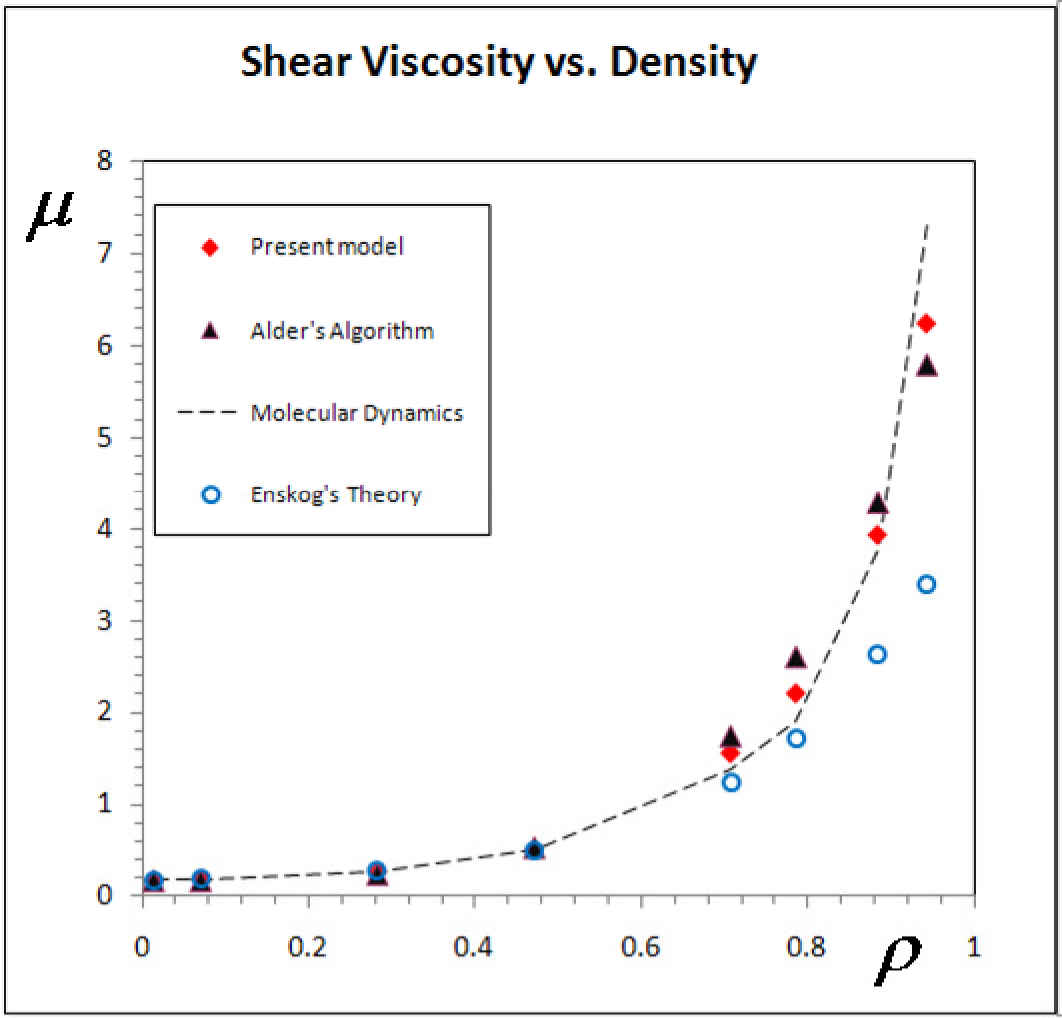
- The velocity during advection depends on denseness of the system.

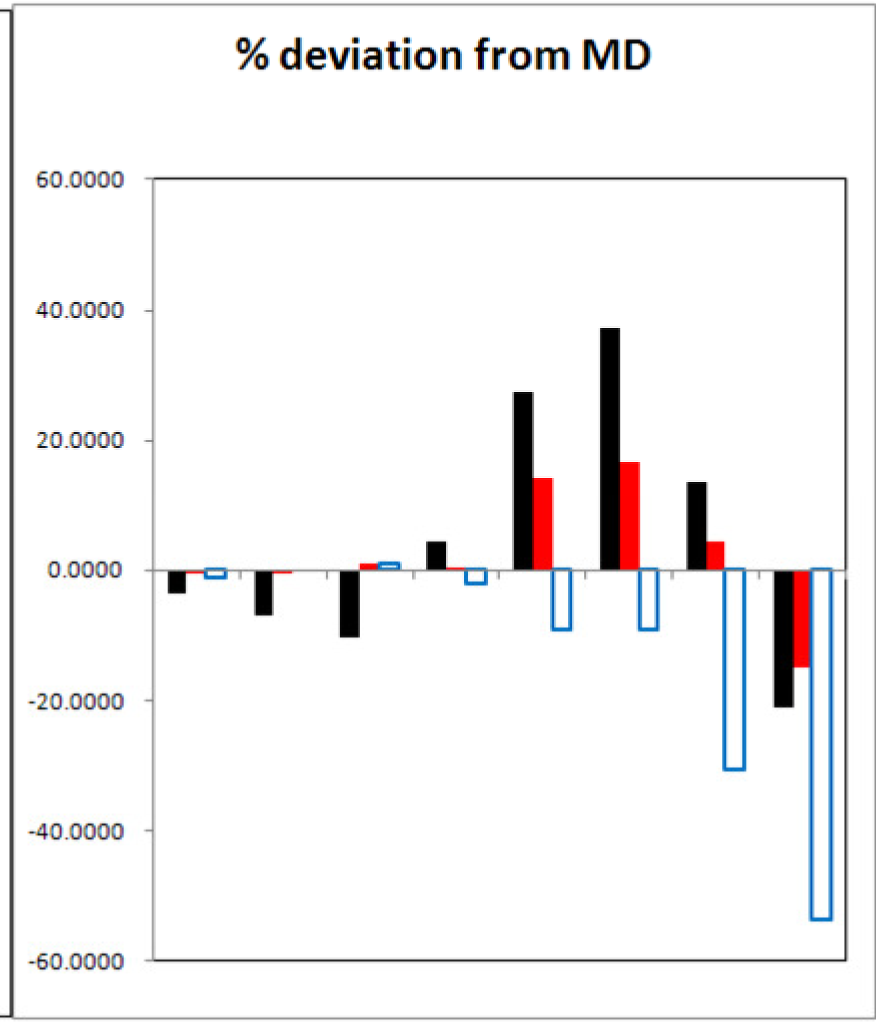
Ref : F.J. Alexander and A.L.Garcia, *Computers and Physics* (1997)

A.Donev , B. J. Alder, and A.L. Garcia, *Phys. Rev. Lett.* 101, 075902 (2008)


DSMC for dilute gases
Alder's Algorithm for Dense gases
DSMC with present model

DSMC of present model (with Boltzmann collision integral)

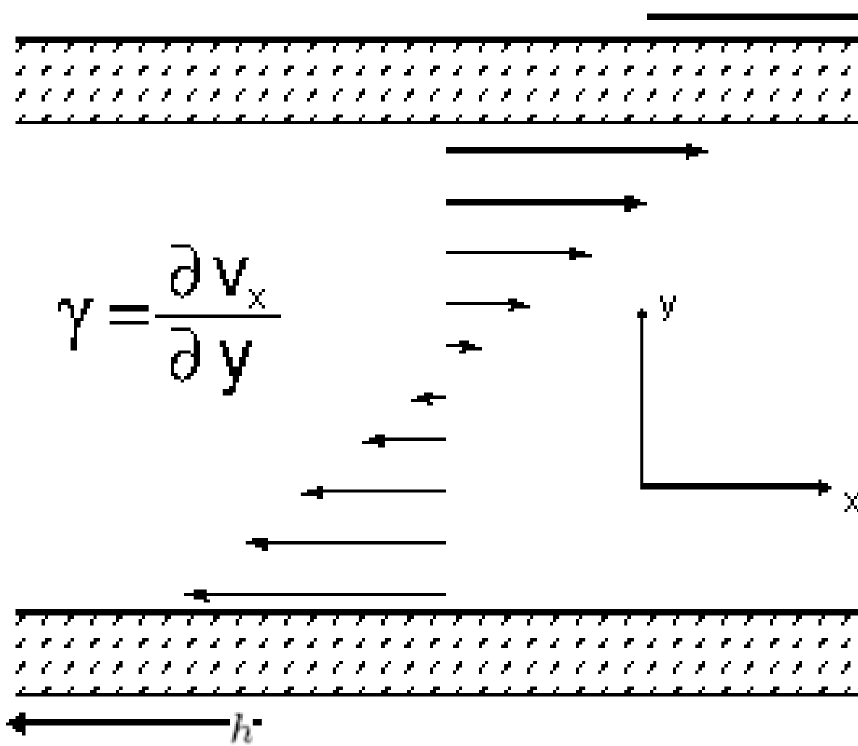




Acknowledgement : Liu Chao & K.S.Kyu (Manuscript under preparation)

Normal stress in uniform Shear

- In order to verify the molecular nature of the model, the variation of normal stress with strain rate predicted by the model is compared with MD [J.F. Lutsko, *Phy.Rev.E* . 58(1). (1998)].



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Normal stress in uniform Shear

- Lee-Edward boundary condition is used and the equation is transformed to local rest frame using :

$$c'_\alpha = c_\alpha - \gamma_{\alpha\beta} x_\beta$$

$$x'_\alpha = x_\alpha - \gamma_{\alpha\beta} x_\beta t$$

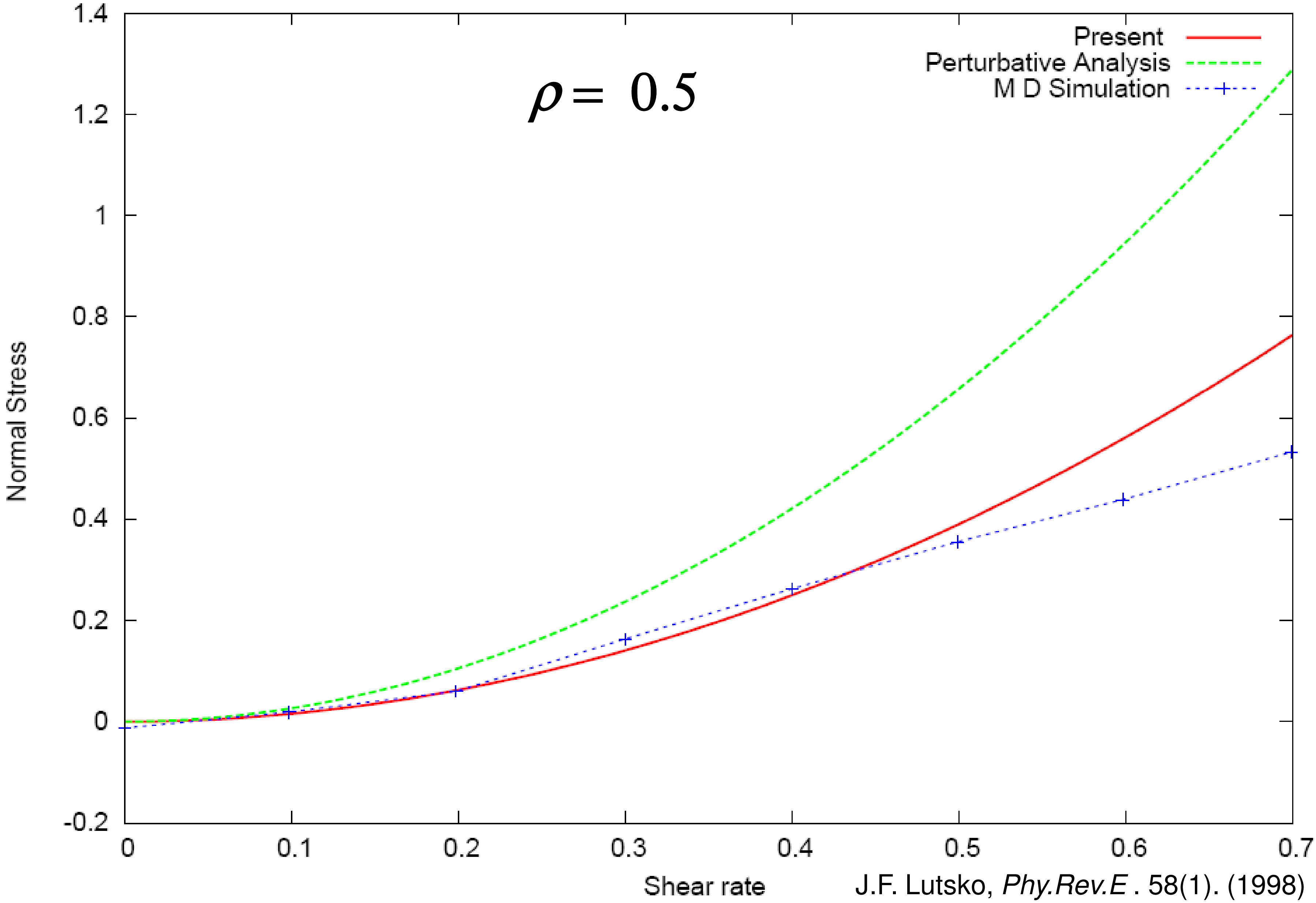
- The transformed equation for the present model is

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_\alpha} \left[(1+\chi) c_\alpha f - \chi u_\alpha f \right] = \frac{f^{eq} - f}{\tau}$$

- By taking appropriate moments,

$$\Psi_1 = 2\,\tau^2 (1+\chi)^2 \rho \left(\frac{k_B T}{m}\right) \quad \text{where} \quad \tau = \frac{5}{16(1+\chi)\sqrt{\pi}}$$

Comparison with MD



J.F. Lutsko, *Phy.Rev.E* . 58(1). (1998)

Present Model – Attractive part

- The model is **extended to multiphase flow** by incorporating an attractive part of the potential is added as a **Vlasov type force**

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \boxed{\frac{1}{\tau}[f^{\mathrm{eq}} - f]} \boxed{- \frac{\partial}{\partial x_\alpha}[\chi^h (c_\alpha - u_\alpha) f]} + \boxed{\frac{\partial f}{\partial c_\alpha} \frac{\partial}{\partial x_\alpha}(\mu^{Att})}$$

BGK Hard sphere Attractive

$$\mu^{Att} = \int \rho(\mathbf{x} + \mathbf{y}) \phi(\mathbf{y}) \mathbf{dy}$$

$$\mu^{Att} \simeq \rho(\mathbf{x}) \int_{\mathbf{r} > \mathbf{d_m}} \phi(\mathbf{r}) \mathbf{dr} + \boldsymbol{\Delta} \rho \frac{1}{6} \int_{\mathbf{r} > \mathbf{d_m}} \mathbf{r^2} \phi(\mathbf{r}) \mathbf{dr} \simeq -\mathbf{2a} \rho(\mathbf{x}) - \kappa \mathbf{d_m^2} \boldsymbol{\Delta} \rho$$

Using gradient theory of interfaces, the parameters a and κ can be related to pair correlation function and the potential using

$$a = -\frac{4\pi}{3} \int_0^\infty g^{eq}(r;\rho) \frac{\partial V(r)}{\partial r} r^3 dr, \qquad u_2 = \frac{4\pi}{15} \int_0^\infty g^{eq}(r;\rho) \frac{\partial V(r)}{\partial r} r^5 dr.$$

Ref: Kikkinides et al *Phy.Rev.E.* (2010)

Conservation Equations (with attractive part)

- On talking moments, the present model with the attractive terms, leads to the following mass and momentum conservation equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha}(\rho u_\alpha) = 0$$

$$\partial_t (\rho u_\beta) + \partial_\alpha \left[p^{\mathrm{Id}} \delta_{\alpha\beta} + \rho u_\alpha u_\beta + (1+\chi)\ \sigma^{(\mathrm{K})}_{\alpha\beta} \right] + \partial_\beta p^{\mathrm{E}} + \underbrace{\partial_\alpha \left(d_m^2 \kappa \, \partial_\beta \rho \, \partial_\alpha \rho \right)}_{\text{VDW Stress}} = 0$$

$$p^{\mathrm{E}} = p^{\mathrm{NID}} - \rho a d_m^2 \kappa \nabla^2 \rho - \frac{1}{2} a d_m^2 \kappa |\nabla \rho\ |^2$$

Summary of present model

- Accounts for non-ideal effects by generalization of propagation velocity; retains BGK collision term.
- Has a valid *H*- Theorem
- Molecular behavior is shown by DSMC and by comparison with MD.
- Attractive term added using Vlasov type force.
- Correct conservation equations

Numerical Scheme – Discrete velocity lattice

The present model is given by

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{1}{\tau}[f^{\mathrm{eq}} - f] - \frac{\partial}{\partial x_\alpha}[\chi^h (c_\alpha - u_\alpha) f] + \frac{\partial f}{\partial c_\alpha}\frac{\partial}{\partial x_\alpha}(\mu^{Att})$$

In a discrete velocity lattice,

$$\frac{\partial f_i}{\partial t} + C_{i\alpha} \frac{\partial f_i}{\partial x_\alpha} = \frac{1}{\tau}[f_i^{\mathrm{eq}} - f_i] \underbrace{- \frac{\partial}{\partial x_\alpha}[\chi^h (C_{i\alpha} - u_\alpha) f_i]}_{F_i^h} \underbrace{- \frac{f_i^{\mathrm{eq}} C_{i\alpha}}{T_0}\frac{\partial}{\partial x_\alpha}(\mu^{Att})}_{F_i^{Att}}$$

Note : $\tau = \dfrac{\nu}{(1+\chi^h)\left(\frac{k_B T}{m}\right)}$

Numerical Scheme

The development and testing of the scheme is initially done in 1-D, later it is extended to 3D.

$$f_i(x+C_{ix}\Delta t, t+\Delta t) - f_i(x,t) = \frac{\Delta t}{2\tau}[J(x+C_{ix}\Delta t, t+\Delta t) + J(x,t)] + \frac{\Delta t}{2}[F_i(x+C_{ix}\Delta t, t+\Delta t) + F_i(x,t)]$$

$$g_i := f_i - \frac{\Delta t}{2\tau} J_i - \frac{\Delta t}{2} F_i$$

$$\boxed{g_i(\mathbf{x} + \mathbf{C}_i\Delta t, t+\Delta t) - g_i(\mathbf{x}, t) = 2\beta(g_i^{eq} - g_i) + 2\beta\tau[F_i(\mathbf{x}, t)]}$$

$$\rho(g) = \rho(f)$$

$$\rho u_\alpha(g) = \rho u_\alpha(f) - \frac{\Delta t}{2}\sum F_i C_{i\alpha}$$

$$P_{\alpha\alpha}(g) = P_{\alpha\alpha}(f) - \frac{\Delta t}{2\tau}(P_{\alpha\alpha}^{eq} - P_{\alpha\alpha}) - \frac{\Delta t}{2}\sum F_i C_i^2$$

Note that the above results are valid for any F_i.

Numerical Scheme (1D) – Hard sphere part

Need to represent F_i^h in terms of g_i alone

to get second order accurate explicit scheme.

On Hermite expanding F_i^h, and neglecting higher order terms in u

$$F_i^h \simeq -\partial_x (W_i C_{ix} \overset{h}{\chi} \rho) = -\rho \frac{W_i C_{ix}}{T_0} \partial_x \mu_x^h$$

$$u_x(f) \simeq u_x(g) - \frac{\Delta t}{2} \partial_x(\mu^h) - \frac{\Delta t}{2} \partial_x \mu^{Att}$$

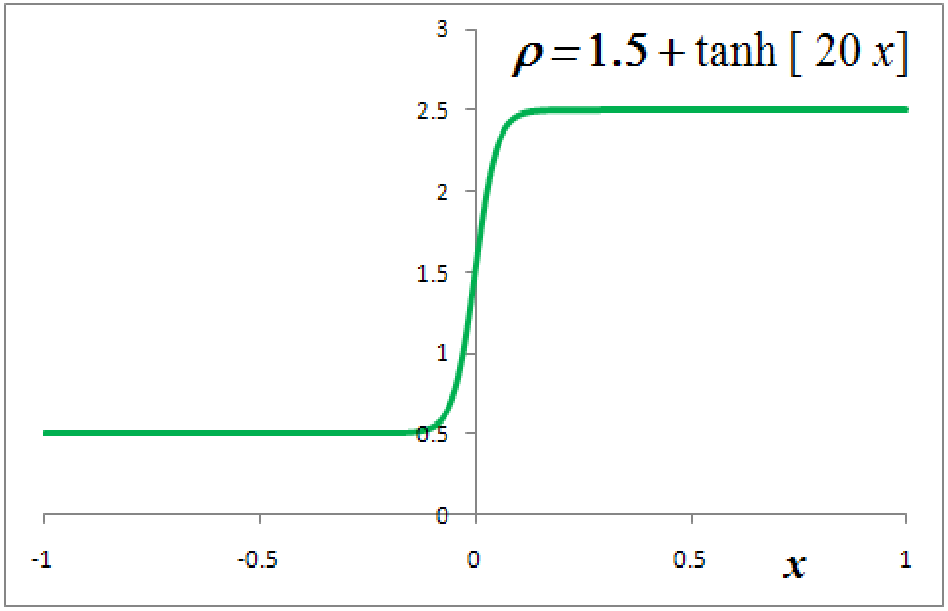
where μ^h is related to χ^h by

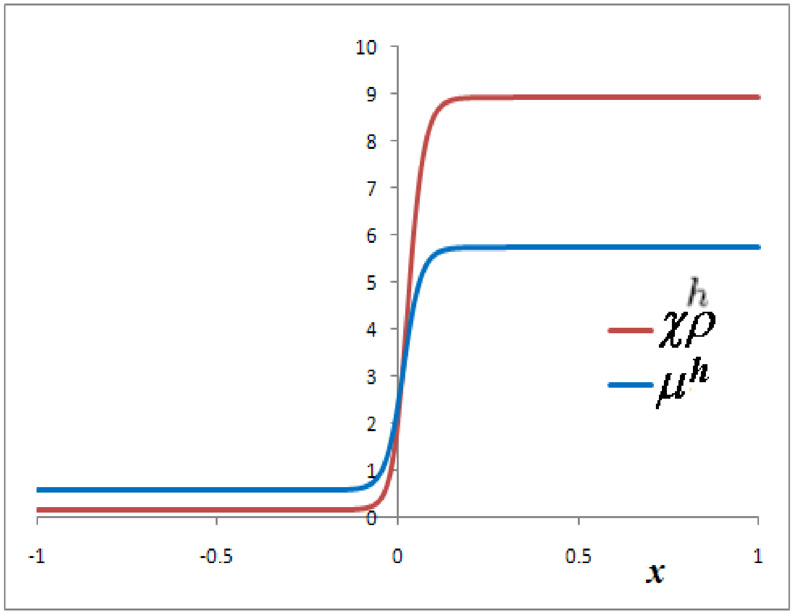
$$\partial_x (\rho \overset{h}{\chi} T_0) = \rho \partial_x \mu^h$$

Gibbs-Duhem relation

- Analytically by the Gibbs-Duhem relation, $\partial_x(\rho\chi^h T_0) = \rho\partial_x\mu^h$
- But in a discrete system where derivative is approximated by finite difference, there is a difference.

Consider the following density profile.

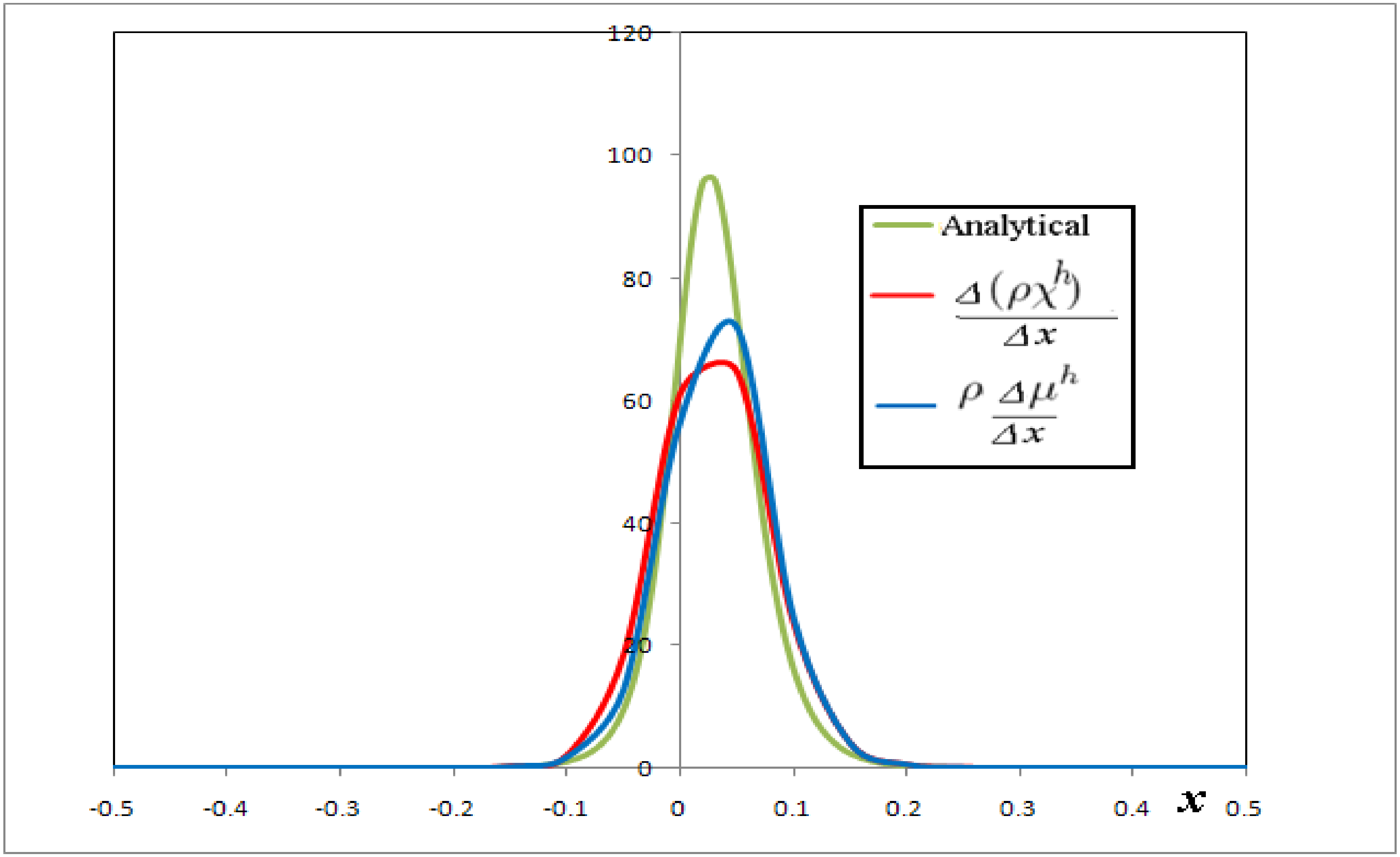




Note that $\chi\rho$ is a much steeper function than μ^h.

Ref : Lee,T. , Fisher, P.F., *Phys. Rev. E,* 74, 046709 (2006).
Wagner, A.J. , *International Journal of Modern Physics B*, 17, pp. 193-196 (2003).

Gibbs-Duhem relation



In a discrete system with low resolution, it can be observed that taking finite difference of μ is more accurate.

Numerical Scheme (1D)

F_i^{Att} is computed at $u = 0$, $F_i^{Att} \simeq= -\rho \frac{W_i C_{ix}}{T_0} \partial_x \mu_x^{Att}$

So the final scheme in 1D is given as

$$\boxed{g_i(x + C_{ix}\Delta t, t + \Delta t) - g_i(x,t) = 2\beta(g_i^{eq} - g_i) - 2\beta\tau\rho\frac{W_i C_{ix}}{T_0}\partial_x \mu}$$

$$u_x(f) = u_x(g) - \frac{\Delta t}{2}\partial_x \mu$$

where $\mu = \mu^h + \mu^{Att}$

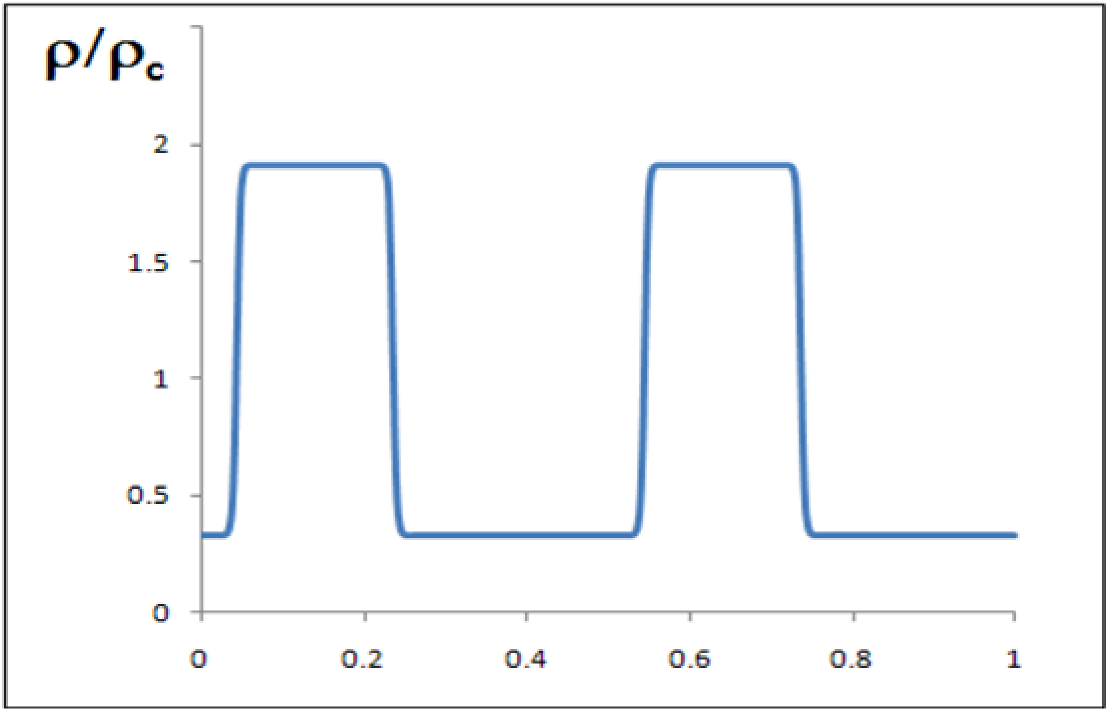
For Carnahan-Starling EOS, $\mu^h = T_0 * \frac{8\frac{\rho b}{4} + 3\left(\frac{\rho b}{4}\right)^2 (\frac{\rho b}{4} - 3)}{(1.0 - \frac{\rho b}{4})^3}$

The density dependence of viscosity is handled by locally computing τ and β using the following virial expansion. This is crucial for stability.

$$\nu = \nu_0 \frac{\rho_0}{\rho}\left(1 + \rho b\left(\frac{5}{8} + \rho b(0.2869 + \rho b(0.1103 + 0.0386\rho b))\right)\right)$$

(Ref. Chapman & Cowling, Mathematical Theory of Non-Uniform gases) :

Results D1Q5



$T / T_c = 0.9$

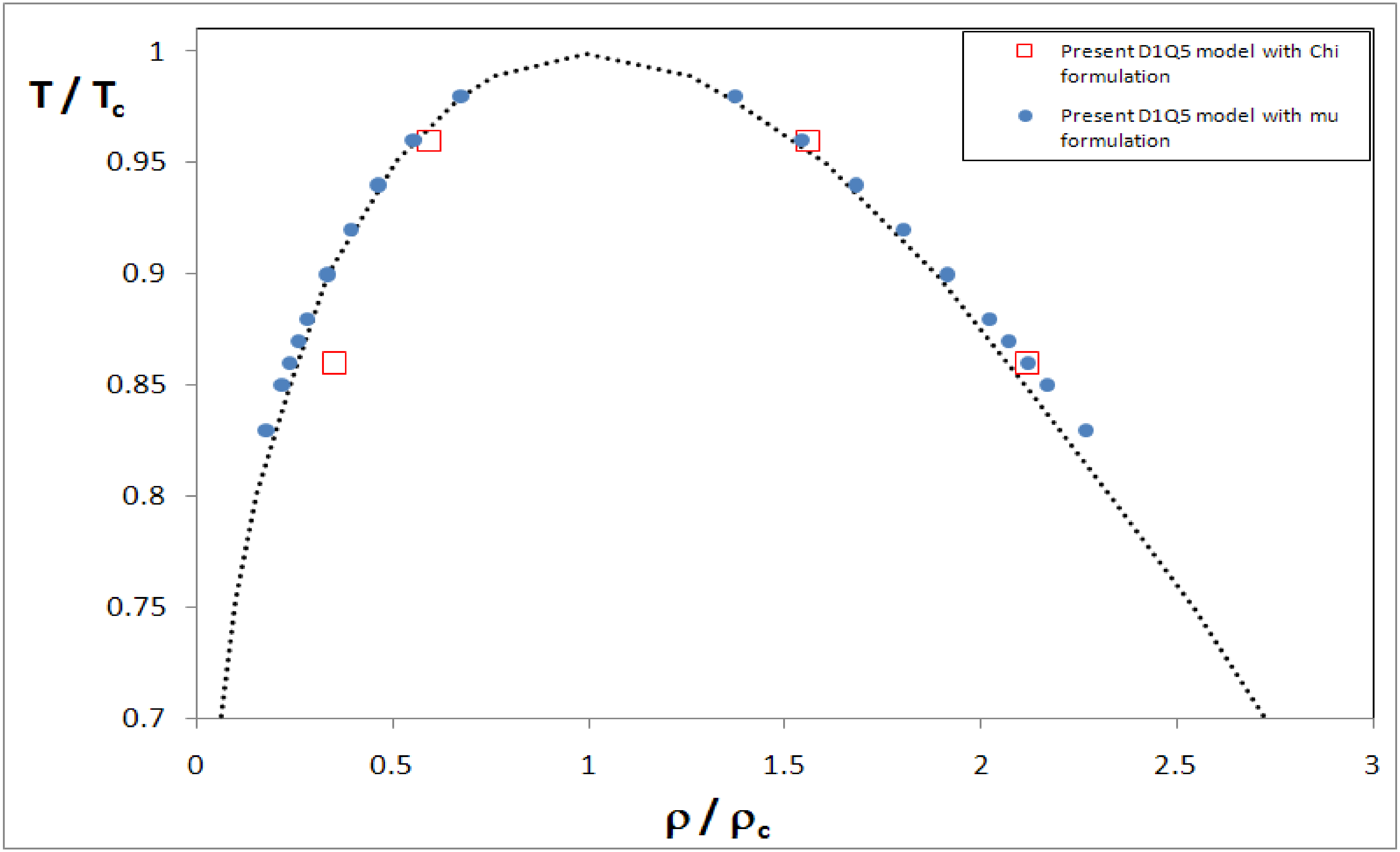
$\rho_0 / \rho_c = 0.94$

$\overline{\kappa} = 0.1$

$\beta = 0.72$

$nx = 350$

Comparison with Maxwell Construction



Extension to 3D

- The 1D scheme is intuitively extended to higher dimensions to lead to

$$g_i(\mathbf{x} + \mathbf{C_i}\Delta \mathbf{t}, \mathbf{t} + \Delta \mathbf{t}) - \mathbf{g_i}(\mathbf{x}, \mathbf{t}) = \mathbf{2}\beta(\mathbf{g_i^{eq}} - \mathbf{g_i}) - \mathbf{2}\beta\tau\rho\frac{\mathbf{W_i C_{i\alpha}}}{\mathbf{T_0}}\partial_\alpha\mu$$

$$u_\alpha(f) = u_\alpha(g) - \frac{\Delta t}{2}\partial_\alpha\mu$$

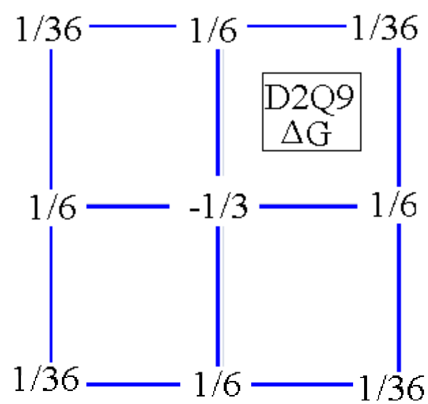
- The gradients and Laplacian are computed in an Isotropic fashion.

- The periodicity of ρ , μ and f are ensured (including at the edges and corner node)

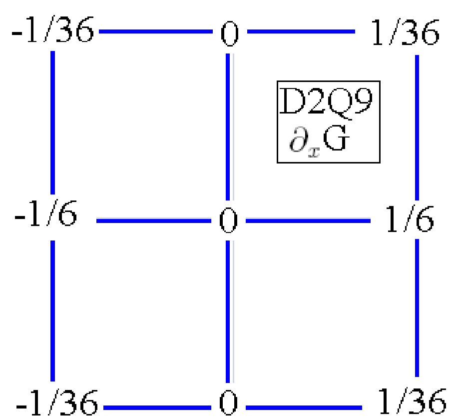
- Equilibrium is currently entropic (for isothermal). A scheme with energy conservation is under development

Gradient and Laplacian calculation

$$\Delta G = \frac{2}{T_0 \Delta t^2}\left(\sum_{i=1}^{N} W_i\, G(\boldsymbol{x} + \boldsymbol{C}_i \Delta t, t) \; - G(x,t)\right) + O(\Delta t^2)$$

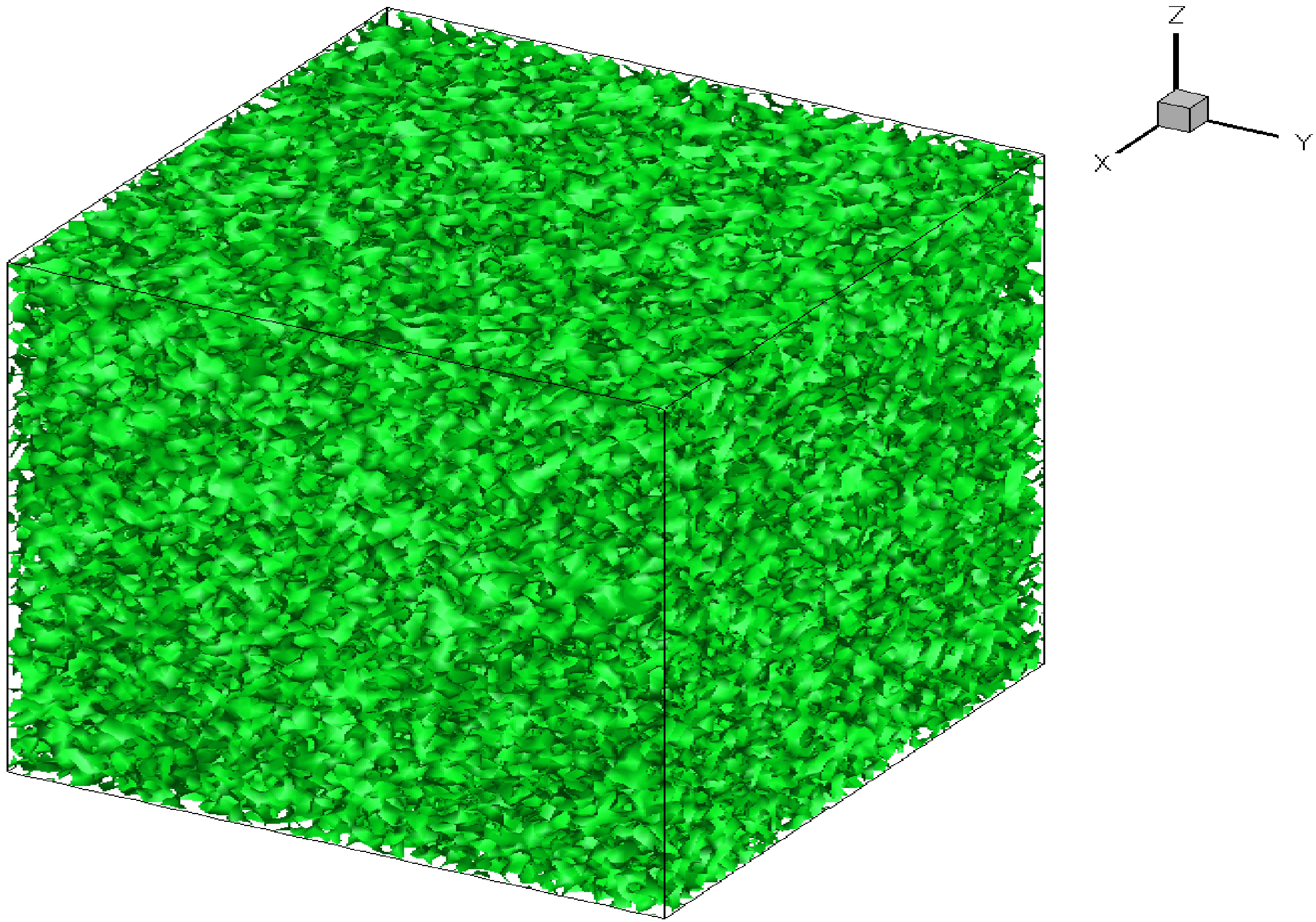


$$\partial_\alpha G = \frac{1}{T_0 \Delta t}\left(\sum_{i=1}^{N} W_i\, C_{i\alpha} G(\boldsymbol{x} + \boldsymbol{C}_i \Delta t, t\right) + O(\Delta t^2)$$

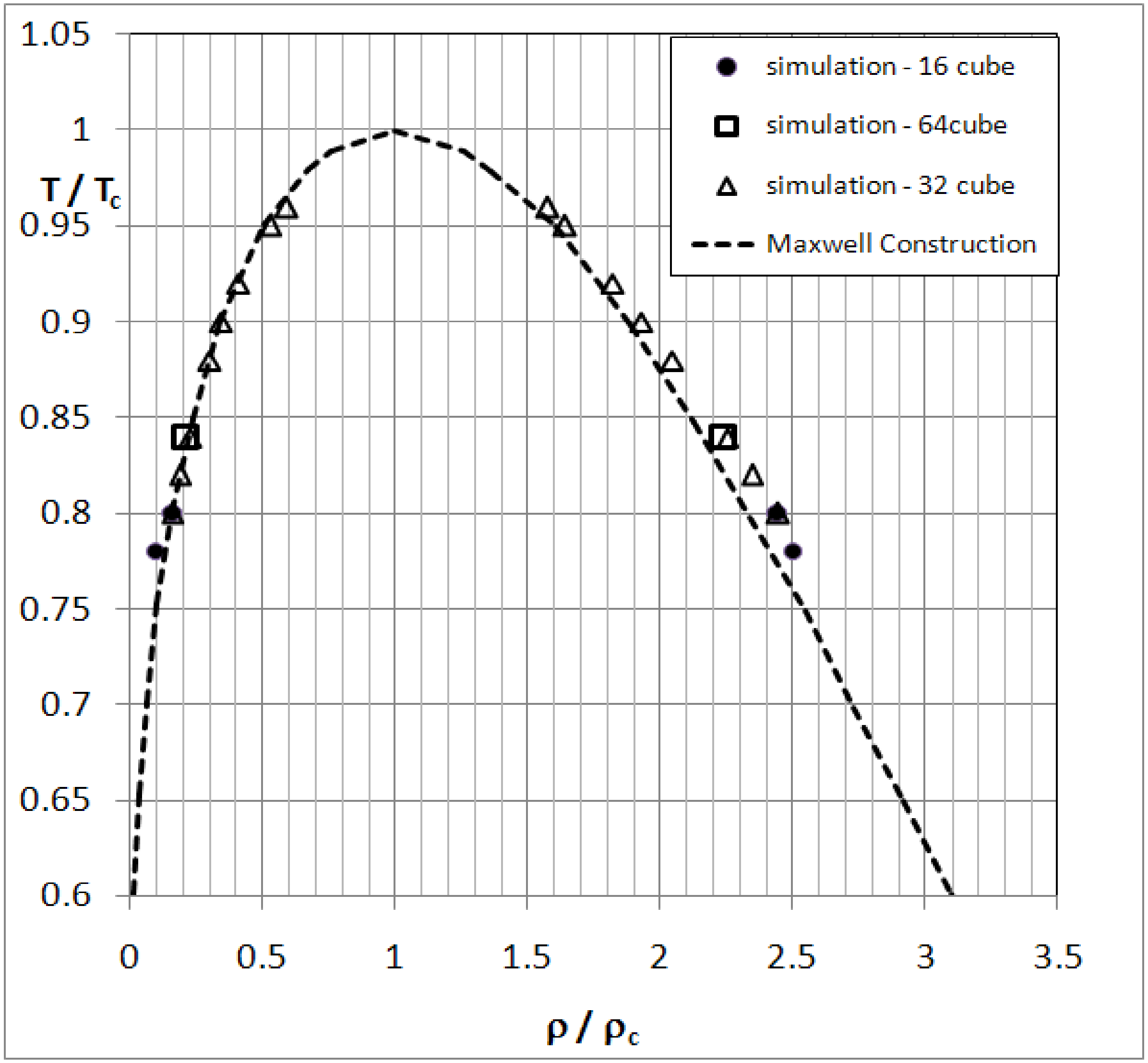


Results from 3D (D3Q27) simulation

Evolution of an iso-surface of density for condensing bubble in periodic domain



Comparison to Maxwell construction



Conclusions

- The proposed extension to BGK-Boltzmann equation for dense gases by generalization of the propagation velocity has been assessed by DSMC and comparison with MD

- The Gibbs-Duhem relation has been exploited to obtain better discretization.

- The density dependence of viscosity has been accounted for and is seen to be important for stability of the scheme.

- The Numerical scheme developed has been successful in simulating condensation in a 3D periodic domain.

- The current numerics are stable upto a density ratio 20 and reproduce Maxwell construction, with a naïve construction.

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