## DSFD 2010 - Rome Italy

Tutorial Title

# Understanding the Nature of Lattices via Symmetry

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Exa CORPORATION

# Contents

# Part 1: Basic (Bottom-Up) Starting Point

Giving a “realizable” micro-dynamic many-body system below,

1.A finite set of velocity values, $\vec{v} \in \{\vec{c}_i;\ i = 1, 2, \cdots, b\}$

2.Corresponding particle density distribution per velocity,

$$\{ f_i(\vec{x},t),\ i = 1, 2, \cdots, b\}$$

3.Interactions obey the usual conservation laws of mass, momentum and energy

Dynamic process is given by a Boltzmann-like equation

$$\partial_t f_i(\vec{x},t) + \vec{c}_i \cdot \nabla f_i(\vec{x},t) = \Omega_i$$

**What macroscopic properties can it recover by such a simple model?**

*Discrete velocity orientations is considered here, instead of spatial (or temporal) discreteness*

*LG/LB may be viewed as having collisions (interactions) occurring on a discrete lattice*

- All hydrodynamic moments are given by discrete summations

$$\left\langle \vec{c}_i^{\,n} \right\rangle (\vec{x},t) \equiv \sum_i \underbrace{\vec{c}_i \ldots \vec{c}_i}_{n} f_i(\vec{x},t)$$

- Hydrodynamics pertains to the first 2 (and trace of 3rd) conserved moments:

$$\partial_t \left\langle \vec{c}_i^{\,n} \right\rangle (\vec{x},t) + \nabla \cdot \left\langle \vec{c}_i^{\,n+1} \right\rangle (\vec{x},t) = 0, \quad n = 0, 1, \ldots$$

**Mass conservation,** $\partial_t \rho + \nabla \cdot (\rho \vec{u}) = 0$

**Momentum conservation,** $\partial_t (\rho \vec{u}) + \nabla \cdot \overleftrightarrow{\Pi} = 0$

**……**

$$\rho = \left\langle \vec{c}_i^{\,0} \right\rangle, \quad \rho \vec{u} = \left\langle \vec{c}_i^{\,1} \right\rangle, \quad \ldots$$ hydrodynamic variables

$$\overleftrightarrow{\Pi} = \left\langle \vec{c}_i^{\,2} \right\rangle$$ momentum flux tensor

**The central task is to have a "correct" closed form for $\overleftrightarrow{\Pi}$,**
**in terms of hydrodynamic variables, as in the continuum physics**

## *Review (Chapman-Enskog):*

- Local conservation dictates that equilibrium distribution is a function of hydrodynamic variables only,

$$f_i^{eq} = g(\rho, \vec{u}, \theta)$$

- Moments expressed in expansions of distribution near equilibrium,

$$f_i = f_i^{eq} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \cdots, \qquad \varepsilon \sim \tau\omega_h$$

$$\overleftrightarrow{\Pi} \equiv \left\langle \vec{c}_i^{\,2} \right\rangle = \left\langle \vec{c}_i^{\,2} \right\rangle^{(eq)} + \left\langle \vec{c}_i^{\,2} \right\rangle^{(1)} + \left\langle \vec{c}_i^{\,2} \right\rangle^{(2)} + \cdots$$

- It amounts to recovery of equilibrium moment tensors up to desired orders,

$$f_i^{(m)} \sim -\varepsilon\tau(\partial_t + \vec{c}_i \cdot \nabla) f_i^{(m-1)} \sim [-\varepsilon\tau(\partial_t + \vec{c}_i \cdot \nabla)]^m f_i^{eq}$$

$$\Rightarrow \left\langle \vec{c}_i^{\,2} \right\rangle^{(m)} \sim \left\langle \vec{c}_i^{\,2+p} \right\rangle^{(eq)}, \quad p = 0, 1, \ldots, m$$

Momentum Stress tensor:

$$\overleftrightarrow{\Pi} \equiv \left\langle \vec{c}_i^{\,2} \right\rangle = \left\langle \vec{c}_i^{\,2} \right\rangle^{(eq)} + \left\langle \vec{c}_i^{\,2} \right\rangle^{(1)} + \left\langle \vec{c}_i^{\,2} \right\rangle^{(2)} + \cdots$$

Leading orders (*for ideal-gas of purely local elastic interactions*):

Euler: $$\left\langle \vec{c}_i^{\,2} \right\rangle_{\alpha\beta}^{(eq)} = \rho\theta\,\delta_{\alpha\beta}$$

Navier-Stokes: $$\left\langle \vec{c}_i^{\,2} \right\rangle_{\alpha\beta}^{(1)} = -2\nu S_{\alpha\beta}, \quad \nu = \tau\theta$$

*Linear relationship between tress and strain (Newtonian fluids)*

2nd order: $$\left\langle \vec{c}_i^{\,2} \right\rangle_{\alpha\beta}^{(2)} = -2\nu \tfrac{D}{Dt}(\tau S_{\alpha\beta})$$

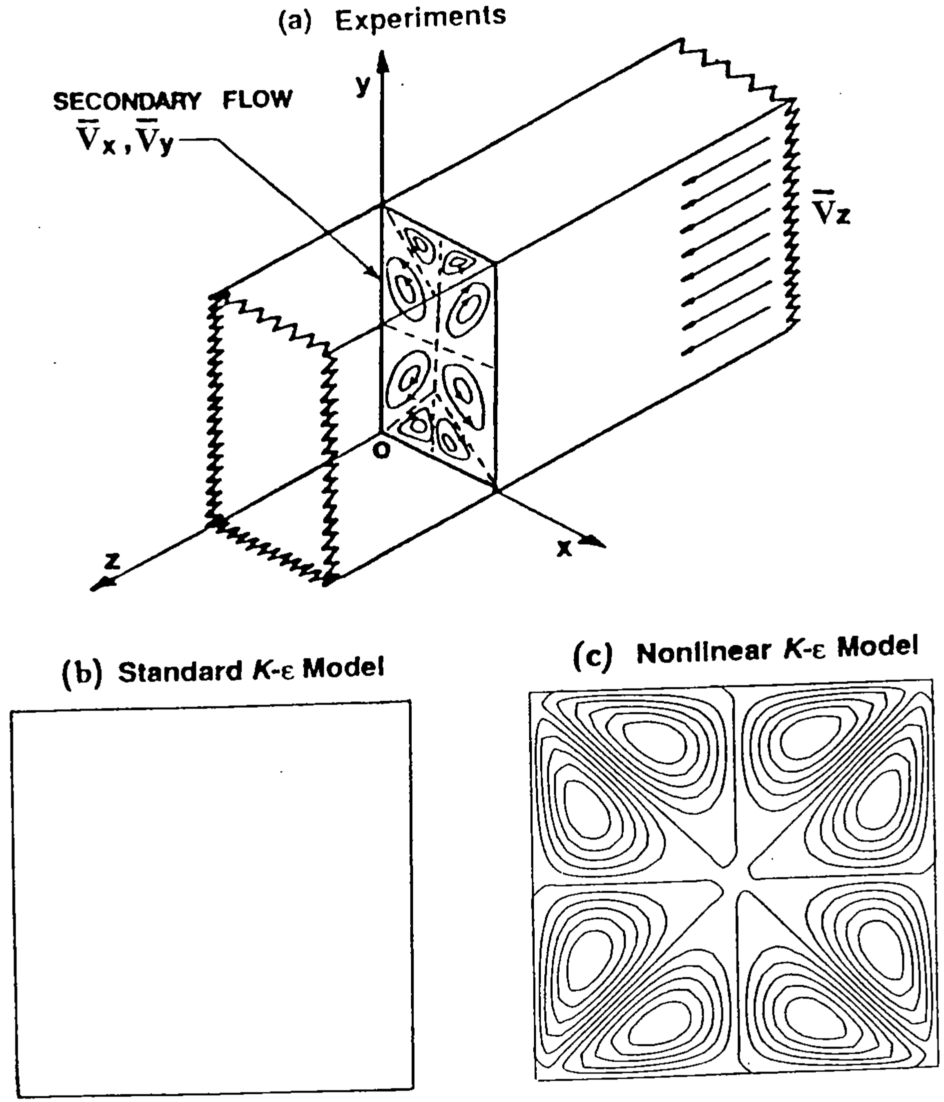
$$-2\tau^2[2(S_{\alpha\gamma}S_{\gamma\beta} - \tfrac{1}{d}\delta_{\alpha\beta}S_{\gamma\delta}S_{\gamma\delta}) - (S_{\alpha\gamma}\Omega_{\gamma\beta} + S_{\beta\gamma}\Omega_{\gamma\alpha})]$$

*Wave-like effect:*

$$\tau\partial_{tt}u + \partial_t u = \nu\nabla^2 u$$

*Yakhot et al, 07*

# Secondary flow in turbulence



## ***Theorem (Fundamental Condition):***

*Equilibrium moments up to* ***(2n)***$^{th}$ ***order*** *recover their continuous Boltzmann counter parts if its lattice velocity set satisfies,*

$$E^{(2n)} \equiv \sum_i w_i \underbrace{\vec{c}_i \vec{c}_i \cdots \vec{c}_i}_{2n} = \theta^n \Delta^{(2n)}$$

$\Delta^{(2n)}$ *is the (2n)*$^{th}$ *rank isotropic tensor*

Properties:

1. $\Delta^{(2n)}$ has a "Gaussian form": Made of symmetric n-products of $\Delta^{(2)}$,

   Eq., $\Delta^{(4)}_{\alpha\beta\gamma\eta} \equiv \Delta^{(2)}_{\alpha\beta}\Delta^{(2)}_{\gamma\eta} + \Delta^{(2)}_{\alpha\gamma}\Delta^{(2)}_{\beta\eta} + \Delta^{(2)}_{\alpha\eta}\Delta^{(2)}_{\beta\gamma}$

   $\Delta^{(2)}_{\alpha\beta} \equiv \delta^{(2)}_{\alpha\beta}$ is the Kronecker delta function.

2. $\Delta^{(2n)} \underbrace{\cdot\cdot\ldots\cdot}_{2n} \underbrace{\vec{V}\vec{V}\ldots\vec{V}}_{2n} = (2n-1)!!\, |\vec{V}^2|^n$ for an arbitrary vector $\vec{V}$

3. $f_i^{eq} = Trunc[w_i \exp[\frac{\vec{c}\cdot\vec{u}}{\theta} - \frac{\vec{u}^2}{2\theta}], O(u^{n+1})]$

# Part 2: Symmetry and Moment Isotropy

**Frisch, Hasslacher and Pomeau (1986); Wolfram (1986):**

*To recover the Navier-Stokes hydrodynamics, $E^{(n)}$ must be isotropic at least to $n = 4$.*

*One finds: Simple square lattice, $n = 2$; Hexagonal lattice, $n = 4$.*

*Why?*

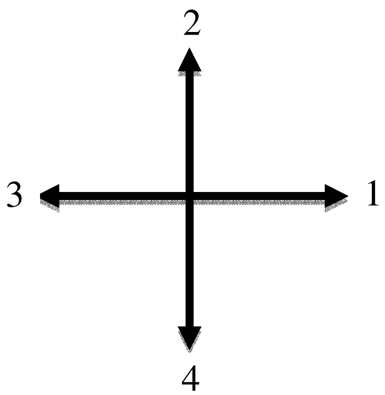
**Def: Degree of rotational symmetry:**

***A 2D object is P-fold rotational symmetric, if it is invariant under rotation angles integer multiple of $2\pi/P$.***

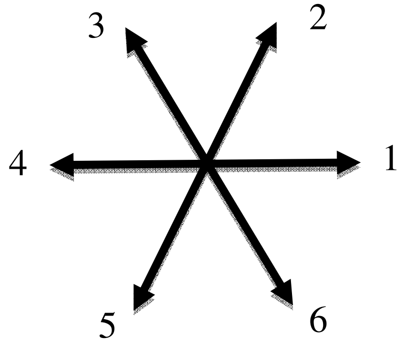
***Theorem***

*If a 2D lattice velocity set is P-fold rotational symmetric, then $E^{(n)}$ is isotropic for $n < P$.*

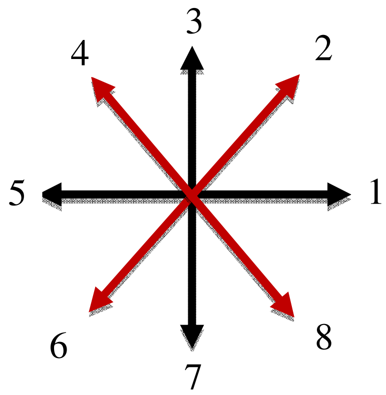
# Velocity of discrete orientations forms a regular "P-gon" {P}:




Square ($P = 4$)



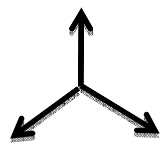

Hexagon ($P = 6$)

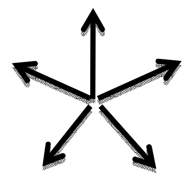



Octagon ($P = 8$)

***P = even : Parity invariant***

***P = odd: Not parity invariant:***





- *triangule {3} and square {4} are 2nd order isotropic,*
  *pentagon {5} and hexagon {6} are 4th order,*
  *{7} and octagon {8} are 6th order,*
  *… … , polygons of infinite orders*
- *{2P} is formed from {P} + its reciprocal {P*} (π/P rotation)*

# Only 5 "regular" discrete velocity orientations (regular polyhedrons in 3D {P,Q}):

*Tetrahedron, {3,3};*

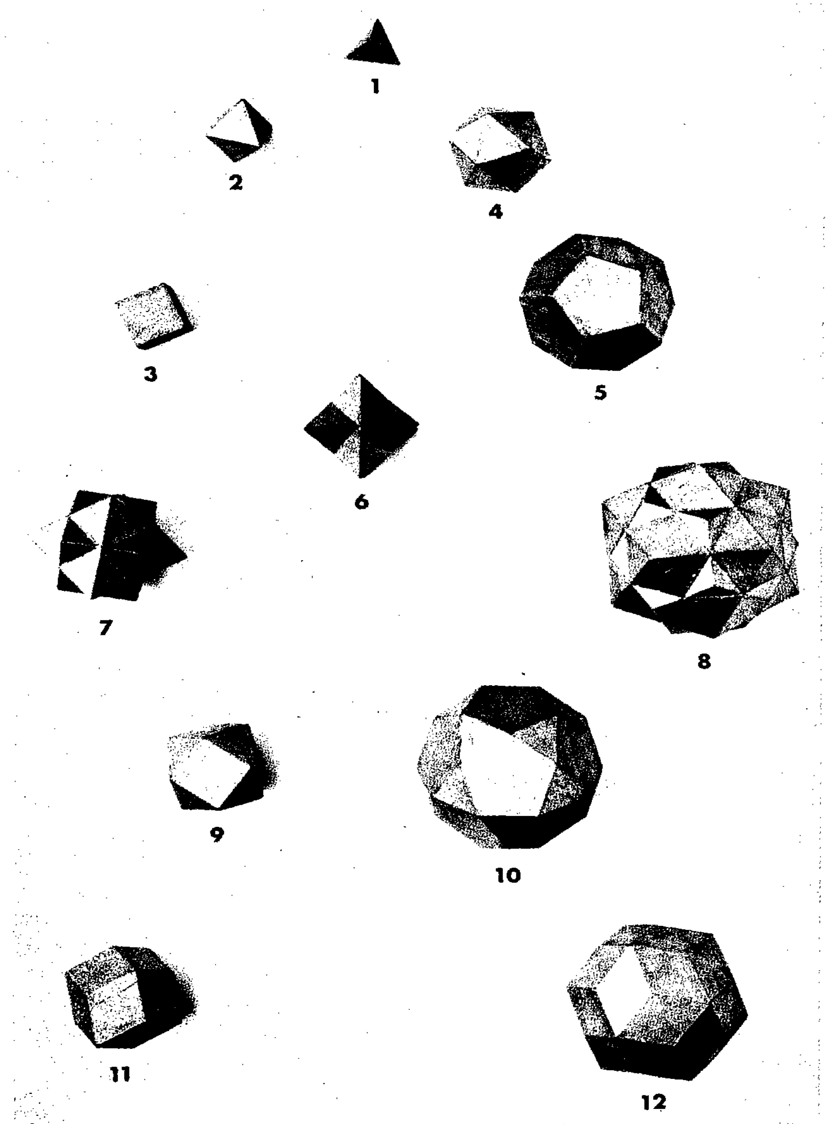
*Octahedron and Cube,*
*{3,4}, {4,3};*

*Icosahedron and Dodecahedron,*
*{3,5}, {5,3}*

*{P,Q} and {Q,P} form a reciprocal pair, having the same symmetry group.*

*Combination of a reciprocal pair forms a quasi-polyhedron, or a rhombic-polyhedron.*

PLATE I




REGULAR, QUASI-REGULAR AND RHOMBIC SOLIDS

## Properties:

1.Observation: {3,4} and {4,3} have no *P*-fold rotation axis > 4; while {3,5} and {5,3} do.

2.Parity invariant polyhedrons {3,4} and {4,3} are 2nd order isotropic, while {3,5} and {5,3} are 4th order isotropic.

3.Combination of a none self-reciprocal pair offer no higher symmetry.

*Icosahedron {3,5} has 12 equal-magnitude vector orientations,*

$$\vec{c}_i \in \{(0,\pm\eta,\pm 1),(\pm 1,0,\pm\eta),(\pm\eta,\pm 1,0)\}$$

- *2nd order tensor isotropy is satisfied with any* $\eta$
- *4th order isotropy obeys,* $\left\langle \vec{c}_i^{\,4} \right\rangle_{\alpha\alpha\alpha\alpha} = 3\left\langle \vec{c}_i^{\,4} \right\rangle_{\alpha\alpha\beta\beta} \quad \alpha \neq \beta$

  *gives* $\eta = 1 + \dfrac{1}{\eta}$

*Series:* $\eta_n = 1 + \dfrac{1}{\eta_{n-1}} = 1 + \dfrac{1}{1 + \dfrac{1}{\eta_{n-2}}} = \ldots., \quad \Rightarrow \quad \eta_n = \dfrac{F_{n+1}}{F_n}$

*"Fibonacci numbers":* $F_0 = F_1 = 1,\ F_{n+1} = F_n + F_{n-1},\ n = 0,1,2\cdots$

## Discrete orientations in higher dimensions: Regular polytopes

1. Single-speed 24-v in 4D: FCHC (or {3,4,3})

$$\vec{c}_i \in \{(\pm1,\pm1,0,0), (\pm1,0,\pm1,0), (0,\pm1,\pm1,0), (\pm1,0,0,\pm1), (0,\pm1,0,\pm1), (0,0,\pm1,\pm1)\}$$

2. Its moment isotropy is satisfied up to 4$^{th}$ order.

3. Projection in 3D gives 18 distinct non-zero velocities in D3Q19,

$$\vec{c}_i \in \{(\pm1,\pm1,0), (\pm1,0,\pm1), (0,\pm1,\pm1), (\pm1,0,0)*2, (0,\pm1,0)*2, (0,0,\pm1)*2\}$$

4. FCHC has a self-reciprocal lattice set, FCHC* *(π/4 rotation in 4D)*:

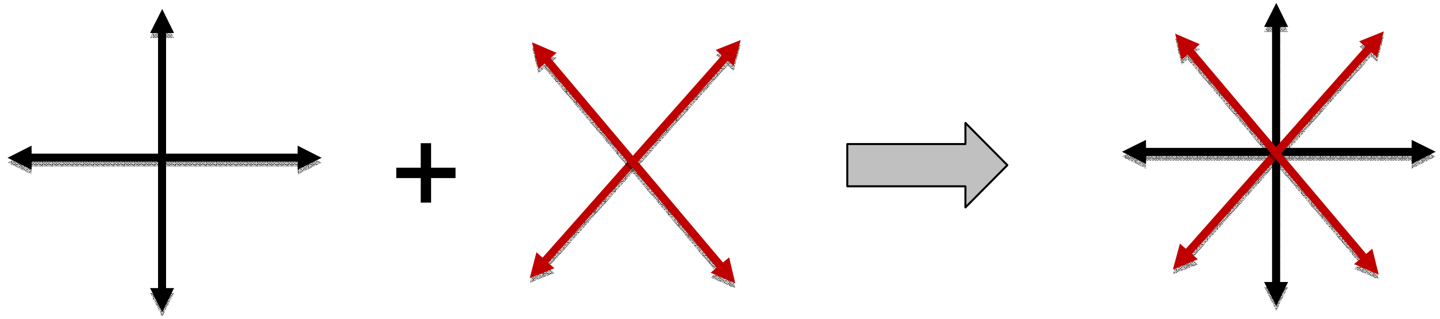
$$\vec{c}_i \in \{(\pm\sqrt{2},0,0,0), (0,\pm\sqrt{2},0,0), (0,0,\pm\sqrt{2},0), (0,0,0\pm\sqrt{2}), (\pm1/\sqrt{2},\ \pm1/\sqrt{2},\ \pm1/\sqrt{2},\ \pm1/\sqrt{2})\}$$

5. Projection of FCHC* in 3D leads to 15 distinct velocities for D3Q15

## Increased symmetry via combination of self-reciprocals

(shapes formed out of a self-reciprocal pair is regular with higher symmetry)

- Square lattices to octagonal lattice:



$2^{nd}$ order isotropic + $2^{nd}$ order isotropic → $4^{th}$ order isotropic

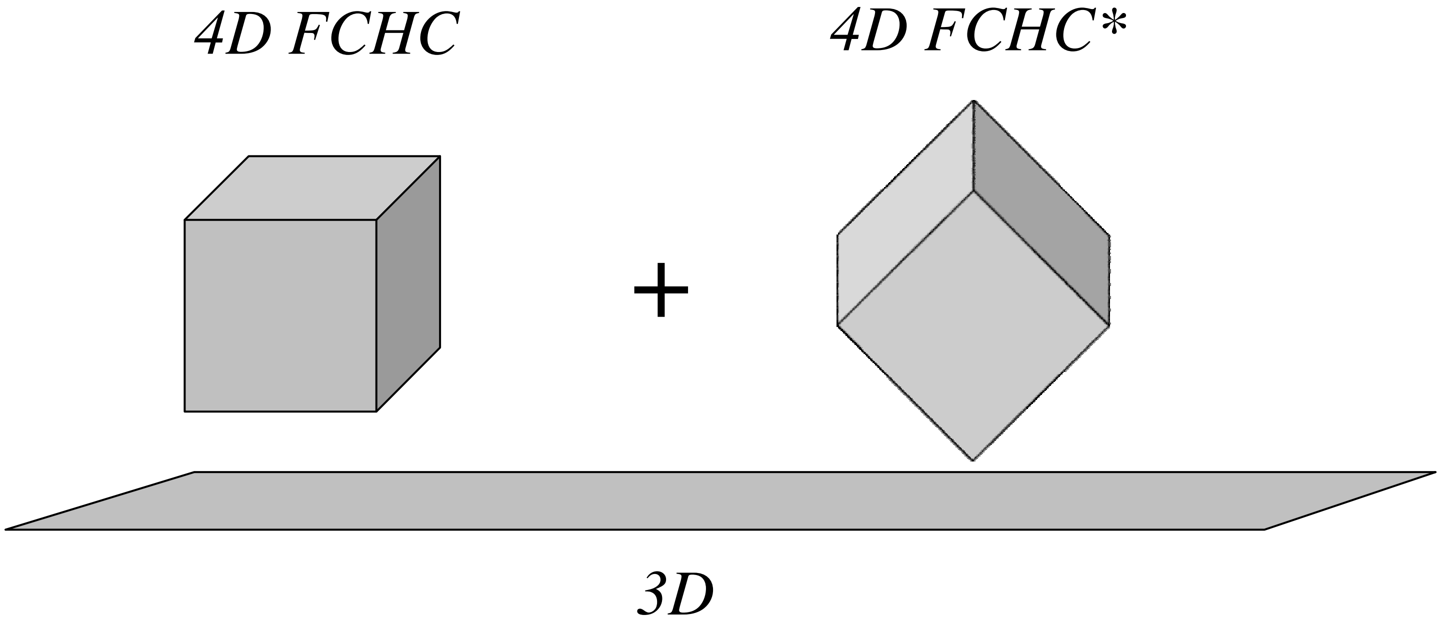
- FCHC with its self-reciprocal:

| | | | | | |
|---|---|---|---|---|---|
| **4D:** | **FCHC** | **+** | **FCHC*** | ⇨ | **FCHC**x2 |
| | $4^{th}$ order isotropic | | $4^{th}$ order isotropic | | $6^{th}$ order isotropic |
| | **24 v** | | **24 v** | | **48 v** |
| **3D:** | **18 v** | **+** | **15 v** | ⇨ | **33 v** |

# Construction of higher isotropy in 3D

*4D FCHC is 4th order isotropic*

*4D FCHC plus its rotation FCHC* gives 6th order isotropy:*




$$\vec{c}_i \in \{(\pm1,\pm1,0), (\pm1,0,\pm1), (0,\pm1,\pm1);\ (\pm1,0,0), (0,\pm1,0), (0,0,\pm1)\}$$

$$\oplus\ \{(\pm\sqrt{2},0,0), (0,\pm\sqrt{2},0), (0,0,\pm\sqrt{2});\ (\pm1/\sqrt{2},\ \pm1/\sqrt{2},\ \pm1/\sqrt{2})\}$$

# Part 3: Rescaling for Integer Cartesian Lattices

**2D lattice:** $\{8\} = \{4\} + \{4^*\}$

$4^{th}$ order moment tensor: $\langle \vec{c}_i^{\,4} \rangle \{8\} = \langle \vec{c}_i^{\,4} \rangle \{4\} + \langle \vec{c}_i^{\,4} \rangle \{4^*\}$ is isotropic

but $\{4^*\}$ has non-integer Cartesian components:

$$\vec{c}_i \in \{(\pm 1/\sqrt{2},\ \pm 1/\sqrt{2})\}$$

Rescaling: $\vec{c}_i \in \{(\pm 1/\sqrt{2},\ \pm 1/\sqrt{2})\} \Rightarrow \vec{e}_i = \sqrt{2}\vec{c}_i \in \{(\pm 1,\ \pm 1)\}$

$$\langle \vec{c}_i^{\,4} \rangle \{4^*\} = \frac{1}{\sqrt{2}^4} \langle \vec{e}_i^{\,4} \rangle \{4^*\} = \tfrac{1}{4} \langle \vec{e}_i^{\,4} \rangle \{4^*\}$$

Forming 8 non-zero integer-component valued velocities in D2Q9:

$$\vec{c}_i \in \{(\pm 1,\ 0),\ (0,\ \pm 1),\ (\pm 1,\ \pm 1) * \tfrac{1}{4}\}$$

**Similar rescaling lead to $4^{th}$ order D3Q15, and $6^{th}$ order D3Q33, etc**

***Property :***

*D-dimensional lattice velocity set of single speed satisfying (2n)<sup>th</sup> order isotropy has an isotropic moment form (for any positive integer n),*

$$G^{(2n)} \equiv \sum_{i=1}^{b} \underbrace{\vec{c}_i \vec{c}_i \cdots \vec{c}_i}_{2n} = bc^{2n} \frac{(D-2)!!}{(D+2n-2)!!} \Delta^{(2n)}$$

$$c = |\vec{c}_i|, \quad i = 1, \ldots, b$$

**A procedure for achieving the fundamental condition:**

1. Rescaling of the single speed $\{\vec{c}_i\}$ in to $J$ multiple speed levels,

$$\{\vec{c}_i\} \;\Rightarrow\; \{\vec{c}_{i,j}\} = \{j * \vec{c}_i\}, \;\; j = 1, 2, \ldots, J$$

2.
$$b \sum_{j=1}^{J} (jc)^{2n} \frac{(D-2)!!}{(D+2n-2)!!} w_j(\theta) = \theta^n$$

$$\Rightarrow \quad E^{(2n)} = \sum_{j=1}^{J} G_j^{(2n)} w_j(\theta) = \theta^n \Delta^{(2n)}$$

# Concluding Remarks

- Symmetry and moment isotropy is an interesting topic in mathematics
- Fundamental for supporting adequate simple discrete micro-systems
- New physical phenomena detected via going in deeper non-equilibrium regimes
- General theorem relating degree of symmetry and order of moment isotropy for higher dimensions (> 2) is to be formulated
- Relevant also for discrete nonlocal interactions
- Extensions for more complex discrete micro-systems,
  - *D-dimensional Ising models of quantized orientations*
  - *Liquid crystals of discrete rod orientations and interactions*
  - *Discrete micro-models for MHD*
  - *Complex and "glassy" fluids of discrete interactions*
  - *Turbulence via discrete micro-models?*

## ***Selected References:***

*1.H. Coxeter (1973) “Regular Polytopes” (Dover publisher).*

*2.S. Wolfram (1986), J. Stat. Phys. **45**, 471-526.*

*3.U. Frisch et al (1987), Complex Systems **1**, 649-707.*

*4.X. Shan, X. Yuan and H. Chen (2006), J. Fluid Mech. **550**, 413-441.*

*5.H. Chen and X. Shan (2008), Physica D **237**, 2003-2008.*

*6.V. Yakhot and C. Colosqui (2007), J. Fluid Mech. **586**, 249.*

*7.H. Chen, S. Orszag, and I. Starolselsky (2007), J. Fluid Mech. **574**, 495-505.*

*8.H. Chen, I. Goldhirsch, and S. Orszag (2008), J. Sci. Compt. **34**, 87-112.*