Lattice Hydrodynamics

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Abstract

Using the combinatorics of two interpenetrating face centered cubic lattices together with the part of calculus naturally encoded in combinatorial topology, we construct from first principles a lattice model of 3D incompressible hydrodynamics on triply periodic three space. Actually the construction applies to every dimension, but has special duality features in dimension three.

1 Introduction

Figure 1: How Cubes Intersect

We construct a particular lattice model of 3D incompressible fluid motion with viscosity parameter. The construction follows the momentum derivation of the continuum model switching to combinatorial topology instead of taking the calculus.
The lattice consists of two interpenetrating face centered cubic lattices which is the crystal structure of NaCl. The lattice defines sodium extreme point cubes with their faces, edges and vertices and chlorine extreme point cubes with their faces, edges and vertices. In this way the lattice of sites organizes a chain complex \( L \) of four vector spaces built from overlapping uniform cubes, faces, edges and sites giving a multi-layered covering of periodic three space. There are two nilpotent operators on \( L \), a duality involution, each of odd degree, and a combinatorial Laplacian. The result of the momentum derivation is an ODE on one degree of freedom.

\[
\frac{\partial \{ V_L \}}{\partial t} = \{ \ast (V_F \cdot v_F) \} + \delta P - \nu \Delta \{ V_L \}, \quad \text{with} \quad \partial \{ V_L \} = 0. \tag{1}
\]

The combinatorics of the combined lattice \( L \) enables a balancing of local and global degrees of freedom required to build the model.

The reference [1] concerns a different approach to models motivated by the infinite heirarchy of cumulant equations arising from the nonlinearity and its relation to quite modern algebraic topology. There was a difficulty there writing a natural physical model in that context. The model here is a more recent attempt to start over from the beginning using traditional combinatorial topology motivated on the one hand by observations of fluids and on the other by the classic breakthrough paper of Leray [2].

The goal of work in progress is to use the model both to derive theory and to compute meaningfully at a given scale those phenomena that can be naively observed.

## 2 The ideas of the construction and definitions

\( L \) denotes the vertices of a regular cubical lattice of edge size \( h \) and of even period in three orthogonal directions (\( x, y, z \)) which are directed. We imagine a fluid uniformly filling and moving through periodic three space.

**Definition 2.1.** \( V_L \): for each site or vertex \( q \) of \( L \), \( V_L(q) \) is a vector at the vertex \( q \) which represents the average velocity of wind or current taken over the cube centered at \( q \) with side length \( 2h \). Namely the integral times \( \frac{1}{8h^3} \). We are assuming the density of particles in the fluid is unity.

**Definition 2.2.** \( V_F, v_F \): For each face \( F \) of side length \( 2h \), \( V_F \) is \( 2hV_L(\text{center point of } F) \) and \( v_F \) is the component of \( V_F \) perpendicular to the oriented \( F \) in the direction defined by the right hand rule.

**Definition 2.3.** Model proposal: We are interested for each oriented \( F \) in the instantaneous transfer of momentum across the face. This is exactly equal to \( \frac{1}{4h^2} \) times the integral over the face \( F \) of (the fluid velocity vector times its orthogonal component to \( F \)). We estimate this average of a product by the product of averages \( V_F \cdot v_F \). This is the closure step in the model which truncates the infinite tower of nonlinear information related to averages of products. When this step proves to be inconvenient the more modern theory of infinity morphisms [1] might be revisited.

**Definition 2.4.** Since \( V_F \cdot v_F \) is a function on oriented faces of side length \( 2h \), we can form \( \delta(V_F \cdot v_F) \), the coboundary of this vector valued function on oriented...
faces. This means a vector valued function whose value on an oriented cube (of side length $2h$) is the sum over its faces of the function on faces, which are oriented by the outward pointing right hand rule.

Definition 2.5. $\ast \delta (V_F \cdot v_F)$ is a lattice vector field, namely a tangent vector valued function on sites, obtained by placing the value of the coboundary for the cube at the center of the cube with a sign that depends on the agreement or not of the orientation of the cube with the chosen orientation of space.

Definition 2.6. $\{ \ast \delta (V_F \cdot v_F) \}$: The $\{ \}$ of a lattice vector field with $(x,y,z)$ components $(a,b,c)$ at site $q$ is the one chain obtained by attaching these values to the three edges with center $q$ and length $2h$ in the $(x,y,z)$ directions oriented in their positive sense. This is the bijection between lattice fields and one chains, formalised in the Theorem below but not reiterated there.

3 Lattice calculus

Definition 3.1. Volume preserving: We are modeling fluids that uniformly fill period three space. We say a lattice vector field $V_L(q)$ is volume preserving iff the 1-chain $\{ V_L \}$ from the definition just stated in the previous section has zero boundary, denoted $\partial$. This means if the edges of length $2h$ are re-oriented so the coefficient of $\{ V_L \}$ is non negative, then at each vertex the sum of the outgoing coefficients is equal to the sum of the incoming coefficients. This accords with Kirchhoff’s laws.

Definition 3.2. Divergence: More generally, the divergence of a lattice vector field $V_L$ is $\partial \{ V_L \}$, where $\{ \}$ is given in the last definition of the previous section.

Definition 3.3. Gradient of a lattice scalar field: For a scalar function of vertices $f$ the gradient $f$ is the 1-cochain whose value on an oriented edge of length $2h$ is the difference of the values at its two endpoints.

Definition 3.4. The Laplacian of a scalar function $f$ of vertices or sites of $L$ is the composition $\Delta f = \partial \delta f$. The value of $\Delta f$ at $q$ is the sum of the values of $f$ at sites $2h$ away from $q$ minus six times the value of $f$ at $q$.

Definition 3.5. Curl of a lattice vector field: If $V_L$ is a lattice vector field, then the curl of $V_L$ is the unique lattice vector field that satisfies $\{ \text{curl} V_L \} = \ast \delta \{ V_L \}$.

Note: The choice of the edge length $2h$ will be formalized in the next section.

4 Lattice topology, the Laplacian and the Hodge decomposition

For global considerations we need to formalize the choice used above to consider only (and all) positive dimensional cells, i.e. edges, faces and cubes, of side length $2h$. So we consider $L_0$, the vector space generated by the vertices or sites of $L$. Then $L_1$, $L_2$, and $L_3$ are defined respectively to be the vector spaces generated by all the oriented edges, faces and cubes of side length $2h$. This gives twice as
many generators as required. This is remedied by imposing the geometric relations 
\((\text{cell, orientation}) = -(\text{cell, opposite orientation})\). Note, as in the figure above, these 
generators can overlap. Also at each site there are exactly three edges of length 
\(2h\) whose midpoint is that site. Thus dimension \(L_1 = 3 \cdot \text{dimension } L_0\). This 
feature of the choice of side length \(2h\) allows one to confound a lattice vector field 
with a one chain, which means a linear combination of oriented edges of length \(2h\).

**Theorem 4.1.** There are canonical isomorphisms \(* : L_0 \leftrightarrow L_3\) and \(* : L_1 \leftrightarrow L_2\). If \(T\) denotes the tangent space to any point of three space there is a canonical isomorphism \(\{\} : L_0 \otimes T \leftrightarrow L_1\). There are maps \(\partial : L_i \to L_{i-1}\) and \(\delta : L_i \to L_{i+1}\) 
satisfying \(\partial \circ \partial = 0\), \(\delta \circ \delta = 0\) and \(* \circ \delta = \partial \circ *, \, * \circ \partial = \delta \circ *\). Define \(\Delta\) in positive 
degrees to be \(\partial \circ \delta + \delta \circ \partial\) which extends the previous definition in degree zero. Then 
there is an “orthogonal” decomposition (called the decomposition of Hodge) of each 
\(L_i\) as \(L_i = \text{im} \partial \oplus \text{im} \delta \oplus \ker \Delta\).

**Remark 4.2.** We note the kernel of \(\Delta\) has rank eight in degrees 0 and 3 and rank 
twenty four in degrees 1 and 2. See Note in the Proof. “Orthogonal” means relative 
to the cellular basis, which is orthonormal.

**Proof.** The graph made of bonds of length \(h\) can be two colored because of the even 
periodicity in all three directions. For a cell of degree one or three of side length 
\(2h\), there is a center point of one color and 2 or 8 vertices in the boundary of the 
opposite color. For a two cell these corner vertices have the same color as the center 
point. In general these extreme point vertices of the cells define the vertices of the 
cell decomposition of the boundary of the cell used to compute the operators \(\partial\) and 
\(\delta\) as is usual in combinatorial topology and Stokes Theorem. Thus a square of side 
\(2h\) has 4 edges of length \(2h\) in its algebraic boundary and a cube of side \(2h\) has six 
faces of edge length \(2h\) in its algebraic boundary, etc.

The duality operator \(*\) relates cells of complementary dimension that intersect 
transversally at their center point. The Hodge decomposition is simple and interesting 
linear algebra valid for any finite dimensional chain complex with positive 
definite inner product with rational or real coefficients and where the second operator 
is defined to be the adjoint of the operator defining the chain complex. The 
kernel of the Laplacian is isomorphic to the homology [or cohomology] of the com-
plex and defines the "harmonic representatives". Harmonic representatives are both 
cycles and cocycles, that is, they belong to the intersection of the kernels of the two 
operators. This follows in the traditional and interesting way, using the positivity 
of the inner product after expanding out \((\Delta V, V)\).

The identities are checked pictorially. The signs in the duality isomorphisms are 
determined by comparing to a global orientation of space. Note the ordering of dual 
cells is not important in this comparison because in our odd dimensional space one 
cell of a dual pair is even dimensional. Otherwise, in even dimensions the order 
counts half of the time.

Note for the Remark: Since one cells have length \(2h\) there eight homology classes 
of vertices. Thus the Laplacian in degree zero has a rank eight kernel. \(\square\)
5 The "potential term" and the "friction term"

The term $\delta P$ in the lattice ODE is meant to cancel the “volume distortion” of the “non linear term” $\{ \ast \delta (V_F \cdot v_F) \}$. So one wants

$$-\Delta P = -\partial (\delta P) = \partial \{ \ast \delta (V_F \cdot v_F) \}$$

In the decomposition of Hodge $\Delta$ preserves the first two factors and is invertible there. Thus we can solve the above and keep the volume preserving property moving forward in time.

For the last term of the ODE promised above, $-\nu \Delta \{ V_L \}$, one assumes the fluid has a linear response to strain which is isotropic. This leads in the volume preserving case to a term proportional to the Laplacian of velocity as explained for example in Landau-Lifschitz "Hydrodynamics".

Combining all of this we get the ODE equation in words, reading first the LHS and then the RHS from right to left: “The rate of change of momentum of a fluid of uniform unit density inside a cube of side length $2h$ is made up of three parts:

i the change of momentum due to internal friction, $\nu \Delta \{ V_L \}$.

ii the change of momentum $\delta m$ inside the cube created by a potential force of the fluid acting on itself. The potential $P$ satisfies $\{ \delta m \} = \delta P$ where $P = \Delta^{-1} (\partial \{ \ast \delta (V_F \cdot v_F) \})$.

iii the change of momentum inside the cube due to a net transfer of momentum across the surface of the cube, $\{ \ast \delta (V_F \cdot v_F) \}$.

Thus,

$$\frac{\partial \{ V_L \} }{\partial t} = \{ \ast \delta (V_F \cdot v_F) \} + \delta P - \nu \Delta \{ V_L \}, \text{ with } \partial \{ V_L \} = 0. \quad (2)$$

References

[1] Sullivan, Dennis. “3D Incompressible Fluids: Combinatorial Models, Eigenspace Models, and a Conjecture about well-posedness of the 3D zero viscosity limit” Journal of Differential Geometry 97.1 (2014): 141-148.

[2] Leray, Jean. “Sur le Mouvement d’un Liquide Visqueux emplissant l’Espace.” Acta Mathematica 63.1 (1934): 193-248.