Lattice Hydrodynamics

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1 Overview

We construct two canonical lattice models of 3D incompressible hydrodynamics on triply periodic three space with periods in each direction the same power of two.

This is based on a "lattice vector calculus" for a special collection of bigger k-cubes inside the cubical decomposition of periodic three space of grid step h. By considering all lattice points plus all edges, faces and cubes of edge size 2h one finds a new discrete version of vector calculus which works nicely. One should note these elements overlap consisting as they do of eight different cubical decompositions of edge size 2h all related by translations in the various directions by h.

This idea for the lattice hydrodynamics begins with the known impossibility to have a finite dimensional version of vector calculus that includes a discrete version or model of differential forms with exterior d and the exterior product which simultaneously satisfies graded commutativity, associativity and the product rule for exterior d.

This means the **same** discretization method applied to different but equivalent versions of NSE at the continuum level might well be fundamentally **different** when the identities used to prove the equivalence at the continuum level do not all hold for the discretization being used.

We do not derive the lattice model by directly discretizing some particular writing of the NSE, but rather we first simply write momentum transfer and creation or destruction in small cubical regions of fixed edge size 2h. This yields the "momentum model" discussed in detail below. Numerical experiments indicate the nonlinear term in this model pumps numerical energy into the system. Using two scales, coarse and fine, numerical reliability is being improved.

A second model based on the same lattice vector calculus but using the vorticity transport principle when the viscosity is zero leads to the "vorticity model". This interpretation requires a discrete version of the Lie bracket of vector fields mentioned below. The "vorticity" model satisfies, the energy dissipation rate is given by the negative energy norm of the vorticity and seems to be more stable numerically than the "momentum" model. (from numerical studies of the two models with D.An,P.Rao and A.Kwon to appear. The physicist Alexandro Cabrero gave one the courage to ignore the momentum principle and use the vorticity transport as a principle instead.)

Besides the critical perspective on discretization mentioned above the new point and the main point is to express the algorithms in terms of an optimal algebraic background for the canonical operations of combinatorial topology that are discrete analogues of the continuum ones exterior d on forms and the divergence operator on multi-vector fields. This optimal setting is the “discrete lattice vector calculus”on the melange of big cubes mentioned above.

This "lattice vector calculus" has discrete analogs of d and the exterior product on the discrete analogue of differential forms denoted δ and "wedge" acting on the cochains.

The "lattice vector calculus" also has discrete analogs of the exterior product of multi-vector fields and its divergence operator ∂ (using any volume form up to scale) whose discrete analogue is the exterior product and its boundary operator denoted "wedge" and ∂ acting on chains.

These products satisfy by construction graded commutativity and associativity but δ does not satisfy the product rule , that is, it is not a first order derivation, as is its continuum analogue d. Thus the product rule for δ acting on the exterior product of cochains is deformed.

Also ∂ is not a second order derivation of its exterior product as is its continuum analogue, where the deviation from being a first order derivation of the exterior product defines a Lie bracket on multivector fields, including the Lie bracket of vector fields.

One takes the deviation of ∂ from being a derivation on the exterior product of chains, called the bracket and denoted [,] to be the **discrete version of the Lie bracket of vector fields** , one chains being the discrete analogue of vector fields, given our volume form. ∂ is by a derivation of the bracket [,] on chains because $\partial\partial$ equals zero. This bracket [,] defined to be the deviation of ∂ from being a derivation of the exterior product of chains, which in the continuum satisfies the Jacobi identity, now only satisfies Jacobi up to chain homotopy.

Each of these discrepancies is treated by methods of algebraic topology and estimates which justify the discretization of the wedge product of forms and the proposed discretization of the Lie bracket of vector fields in work with R. Lawrence and N. Ranade which will appear in the volume honoring the memory of Sir Michael Atiyah.

Besides the discrete operators **coboundary and boundary** of algebraic topology, the **poincare dual cell** operator plays the role of the Hodge star operator. When cochains and chains are identified using the natural basis the two operators are adjoint and related by conjugation by hodge star.

Exen though the calculus limit is not taken, the derived ODE , “momentum model” for the lattice velocity vector field written in the lattice vector calculus is exactly the Leray form of NSE having the derivative outside the nonlinear term.

The “vorticity model” in this vector calculus language becomes the other familiar form of NSE with the derivative on the inside of the nonlinear term.

So regarding conservation laws at the coarse scale of computation one must choose in this lattice vector calculus between 1) the momentum model with conservation of momentum but with energy being put in by the nonlinear term and 2) the vorticity model where there is dissipation of energy proportional to the energy of vorticity but no explicit momentum conservation.

2 Introduction to the"momentum model"

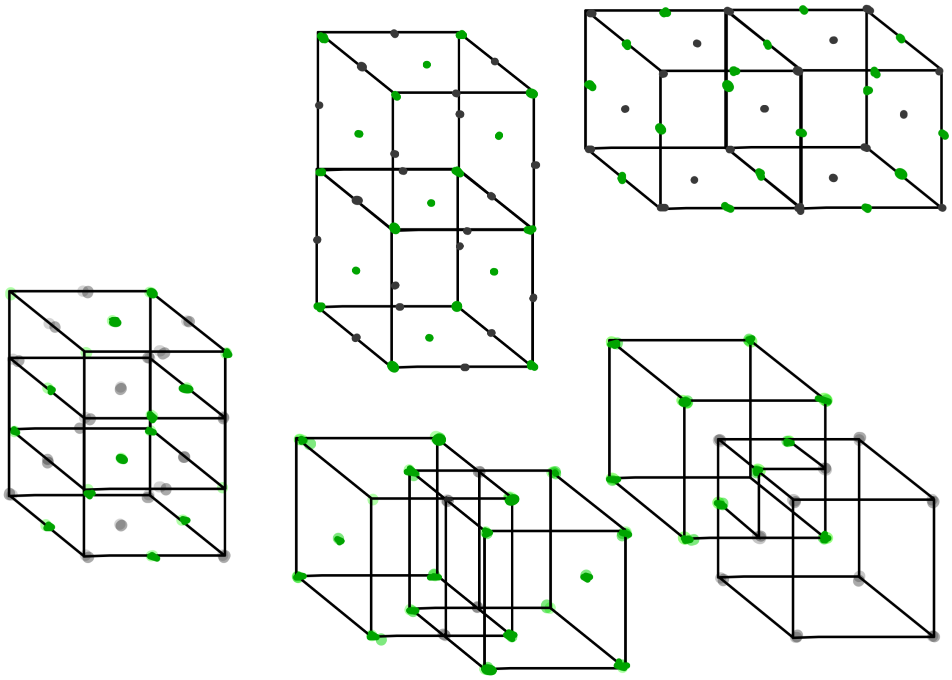

Figure 1: How Cubes Intersect

We construct a particular lattice “momentum” model of 3D incompressible fluid motion with viscosity parameter. The construction follows the momentum derivation of the continuum model using combinatorial topology instead of taking the calculus limit.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 L which is a combinatorial version of the continuum model.

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

The combinatorics of the combined lattice L enables a balancing of local and global degrees of freedom required to build the “momentum”model. The derived ODE is exactly that form of NSE used in the classic paper of Leray. [2] The “vorticity model” which uses the part of lattice vector calculus using vector fields contracted against differential forms will be discussed later. The reference [1] concerns an additional approach to models motivated by the infinite heirarchy of cumulant equations arising from the nonlinearity and its potential relation to quite modern algebraic topology. 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.

3 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.

The lattice vector field, V_L: for each site or vertex q of L, $V_L(q)$ is a three space 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 of velocity times $\frac{1}{8h^3}$. We are assuming the density of particles in the fluid is unity.

The face velocity vectors and face normal components, V_F, v_F: For each face F of side length $2h$, V_F is V_L at the 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.

The model proposal: We are interested for each oriented F in the instantaneous transfer of momentum across the face. This is equal to the product of V_F and v_F.

The derivative outside the nonlinear term: 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) which is the sum over its faces of the function on faces, which are oriented by the outward pointing right hand rule. This being the Stokes theorem in the combinatorial topology context. So this gives the net amount of momentum crossing the boundary of the cube.

The nonlinear term as a lattice vector field: $*\delta(V_F \cdot v_F)$ 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.

The nonlinear term as a one chain: $\{*\delta(V_F \cdot v_F)\}$: 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.

4 Lattice Vector calculus

Volume preserving: We are modeling fluids that uniformly fill periodic 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 ∂. 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 Kirchoff's laws.

Divergence operator: The **divergence** of a lattice vector field V_L is $\partial\{V_L\}$, where $\{\quad\}$ is given in the last paragraph of the previous section.

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.

Laplacian of f : The Laplacian of a scalar function f of vertices or sites of L is the composition $\Delta f = \partial\delta f$. The value of Δf 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.

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

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

5 Lattice topology, the Laplacian and the Hodge decomposition

For global considerations we will formalize in terms of vector spaces the choice used above to consider only (and all) positive dimensional cells, i.e. edges, faces and cubes, of side length $2h$.

Let L_0 denote the vector space generated by the vertices or sites of L. Note they are separated by h not by $2h$. 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 $2h$ and not h.

Actually orientation gives twice as many generators as required . This is remedied by imposing the geometric relations (cell, orientation) = - (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 = three $\cdot$ 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 $2h$. Thus the chain groups decompose as a direct sum over the sites of the exterior algebras on the tangent space of three space at that site. Similarly, the cochains decompose as a direct sum of the exterior algebras of the cotangent spaces at the sites.

This is the main advantage of this model. Indeed, more generally all of the algebra of vector calculus resides at each site. For example, the direct sums of the exterior spaces on the tangent space and the exterior spaces on the cotangent spaces are independently graded commutative associative algebras and become enriched by the boundary and coboundary operators of combinatorial topology. And there are contraction operators between the exterior algebra of chains and the exterior algebra of cochains. Furthermore we have,

Theorem 5.1. *1. There are isomorphisms* $*: L_0 \leftrightarrow L_3$ *and* $*: L_1 \leftrightarrow L_2$.

2. If T denotes the tangent space to any point of three space there is a canonical isomorphism : $L_0 \otimes T \leftrightarrow L_1$ *, sending V to $\{V\}$.defined in section 2.*

3. *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 $* \circ \delta = \partial \circ *$, $* \circ \partial = \delta \circ *$.*

4. *Define Δ in positive degrees to be $\partial \circ \delta + \delta \circ \partial$ which extends the previous definition in degree zero. There is then the "orthogonal" decomposition of each L_i as $L_i = \mathrm{im}\partial \oplus \mathrm{im}\delta \oplus \mathrm{kernel}\Delta$. This, as a lemma about chain complexes with adjoint operators for an inner product is due to Hodge.*

Remark 5.2. *We note the kernel of Δ 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 degree 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 ∂ and δ 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 complex 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 $(\Delta V, V)$. Note the cohomology of L is eight copies of the cohomology of the three torus.

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 are eight linearly independent homology classes of vertices. Thus the Laplacian in degree zero has a rank eight kernel.

□

6 The "potential term" and the "friction term"

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

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

In the decomposition of Hodge, Δ 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.

In computation it is well known this part is more costly by a factor proportional to the inverse of the scale of the scale to the sixth power. Actually closer to the fifth power because we have a sparse matrix inversion problem. Whereas the cost of all of the other terms being local are proportional to the inverse of the cube of the scale.

Remark 6.1. *The mathematician Daniel An has observed in this model one gains a factor of eight in the limitation on scale imposed by the computational budget. This, because the Poisson step in solving for the pressure is done independently on each of the eight 3-cycles or systems of partioning cubes of the model.*

For the friction 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 M of a fluid of uniform density assumed to be unity (so $M = V_L$) 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 δM inside the cube created by a potential force of the fluid acting on itself. The potential P satisfies $P = \Delta^{-1}(\partial\{*\delta(V_F.v_F)\})$.

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

Thus,

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

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.