415

ASTÉRISQUE

2020

SOME ASPECTS OF THE THEORY OF DYNAMICAL SYSTEMS: A TRIBUTE TO JEAN-CHRISTOPHE YOCCOZ

Volume I

Lattice Hydrodynamics

Dennis Sullivan

SOCIÉTÉ MATHÉMATIQUE DE FRANCE

Astérisque
415, 2020, p. 215–222
doi:10.24033/ast.1106

LATTICE HYDRODYNAMICS

by

Dennis Sullivan

In memory of Jean-Christophe Yoccoz

Abstract. — We make use of the combinatorics of two interlocking face centered cubic lattices to make a discrete vector calculus which allows construction of two models of incompressible fluid motion in periodic three space, one based on momentum conservation and one based on the principle of vorticity transport. Without taking the calculus limit, one nevertheless arrives in the vector calculus language to the exact writings of the continuum model, the first due to Jean Leray with the derivative on the outside of the nonlinear term and then the familiar form with the derivative on the inside. Numerical studies show these two models are different at the discrete level.

***Résumé* (Hydrodynamique sur les réseaux).** — Nous utilisons la combinatoire de deux réseaux cubiques à faces centrées sinterpénétrant pour construire un calcul vectoriel discret qui permet la construction de deux modèles de lhydrodynamique incompressible de lespace tridimensionel tripériodique, l'une fondée sur la conservation de l'élan et l'autre sur le principe du transport de la vorticité. Sans passer à la limite différentielle, on arrive néanmoins dans le langage du calcul vectoriel exactement aux formulations du modèle continu, d'abord celle de Jean Leray, où la dérivation agit à l'exterieur du terme nonlinéaire, et ensuite celle plus habituelle où elle agit à l'intérieur. Des études numériques montrent que ces deux modèles diffèrent au niveau discret.

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

2010 Mathematics Subject Classification. — 76A99.
Key words and phrases. — Computational fluid mechanics.

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"

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 multilayered 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

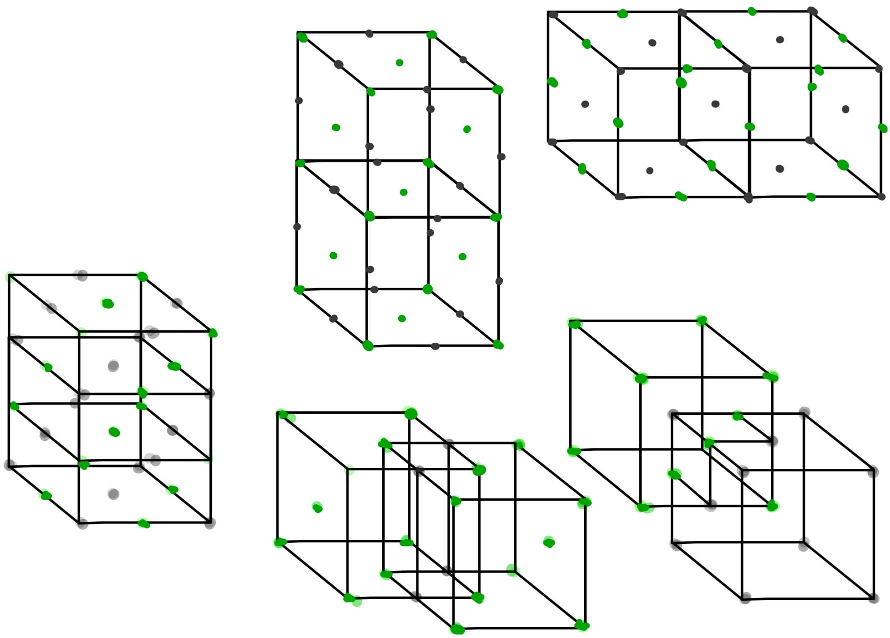

FIGURE 1. How Cubes Intersect

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. [**1**] The "vorticity model" which uses the part of lattice vector calculus using vector fields contracted against differential forms will be discussed later. The reference [**2**] 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