Local Energy Conservation Law for Spatially-Discretized Hamiltonian Vlasov-Maxwell System

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Abstract

Structure-preserving geometric algorithm for the Vlasov-Maxwell (VM) equations is currently an active research topic. We show that spatially-discretized Hamiltonian systems for the VM equations admit a local energy conservation law in space-time. This is accomplished by proving that for a general spatially-discretized system, a global conservation law always implies a discrete local conservation law in space-time when the algorithm is local. This general result demonstrates that Hamiltonian discretizations can preserve local conservation laws, in addition to the symplectic structure, both of which are the intrinsic physical properties of infinite dimensional Hamiltonian systems in physics.

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The dynamics of a collection of charged particles and electromagnetic fields is governed by the well-known Vlasov-Maxwell (VM) equations

\[
\frac{\partial f_s}{\partial t} + v \cdot \nabla f_s + \frac{q_s}{m_s} (E + v \times B) \cdot \frac{\partial f_s}{\partial v} = 0, 
\] (1)

\[
\frac{\partial B}{\partial t} = -\nabla \times E; 
\] (2)

\[
\frac{\partial E}{\partial t} = \nabla \times B - \sum_s \int d\mathbf{v} q_s f_s (\mathbf{x}, \mathbf{v}, t) \mathbf{v}, 
\] (3)

where \(E\) and \(B\) are electromagnetic fields, \(f_s, m_s\) and \(q_s\) are the number density distribution function, mass and charge of the \(s\)'th particle, respectively. Here the permittivity and permeability are set to 1 for simple notation. This set of equations is also a Hamiltonian Partial Differential Equation (PDE), which means that solutions of the equations conserve the symplectic structure and various types of invariants. As one of these invariants, the Hamiltonian itself is conserved, i.e.,

\[
\frac{\partial}{\partial t} \int d\mathbf{x} \left( \frac{E^2 + B^2}{2} + \sum_s \int d\mathbf{v} \frac{1}{2} m_s v^2 f_s (\mathbf{x}, \mathbf{v}; t) \right) = 0. 
\] (4)

For the Vlasov-Maxwell equations and many other Hamiltonian PDE systems, there are also local conservation laws, which can be written in the following form

\[
\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} = 0, 
\] (5)

where \(p\) is a scalar field or a component of a tensor or vector field, and \(\mathbf{u}\) is the flux corresponding to \(p\). As an important example, the local energy conservation law for the Vlasov-Maxwell system reads

\[
\frac{\partial}{\partial t} \left( \frac{E^2 + B^2}{2} + \sum_s \int d\mathbf{v} \frac{1}{2} m_s v^2 f_s (\mathbf{x}, \mathbf{v}; t) \right) + \nabla \cdot \left( \mathbf{E} \times \mathbf{B} + \sum_s \int d\mathbf{v} \frac{1}{2} m_s v^2 \mathbf{v} f_s (\mathbf{x}, \mathbf{v}; t) \right) = 0. 
\] (6)

It can be verified directly by using the Vlasov-Maxwell equations (1)-(3). The conservation law can also be obtained by using Noether’s theorem and the weak Euler-Lagrangian equations. Local conservation laws are more fundamental and practical than global conservation laws, because we often consider systems without global conservations, for example, systems with open boundaries and particle sources. Nowadays, Particle-In-Cell (PIC) simulations are commonly used in the investigation of Vlasov-Maxwell systems,
and advanced structure-preserving geometric algorithms based on variational or Hamiltonian discretization have been developed recently \cite{17-32}. Some of these structure-preserving PIC schemes are able to bound the global energy errors for all simulation time-steps and are effective for solving multi-scale problems \cite{19, 24, 32}. For these algorithms, the corresponding spatially-discretized systems conserve global energy as a consequence of time symmetry admitted by the system. However, as an essential physical property, the discrete local energy conservation has not yet been discussed. If a discrete system has a local conservation law, it implies that at every grid point there is a conservation law, which is much stronger than just one global conservation law for the entire system. There have been some investigations on the discrete local energy conservation law associated with Yee’s FDTD schemes for Maxwell’s equations \cite{33, 34}. However, the local conservation law for discrete particle-field systems is still an unexplored topic. In this paper, we prove a discrete local energy conservation law for the spatially-discretized Vlasov-Maxwell system described in Ref. \cite{24}. This is accomplished by proving in the Appendix a theorem stating that for a general spatially-discretized system, a global conservation law always implies a discrete local conservation law in space-time when the algorithm is local. Here, an algorithm is called local if the time-advance of a field at a grid point or a particle involving only its neighboring grid points and particles. With this theorem, for any geometric spatial-discretizations with local algorithms, we only need to search for global conservation laws and then the corresponding local conservation laws are automatically satisfied. This general result demonstrates that Hamiltonian discretizations can preserve local conservation laws in space-time, in addition to the symplectic structure, both of which are the intrinsic physical properties of many important infinite dimensional Hamiltonian systems in physics.

The idea of structure-preserving spatial discretization of the Vlasov-Maxwell equations can be traced back to Lewis \cite{35} who proposed a spatial-discretized Lagrangian for Vlasov plasmas. Today, modern geometric discretizations for constructing PIC schemes are based on Discrete Exterior Calculus (DEC) \cite{36, 37}, interpolation forms \cite{24, 38, 39} or Finite Element Exterior Calculus (FEEC) \cite{40, 42} to ensure the conservation of charge, the gauge invariance, and the symplectic structure \cite{17, 18, 24, 28, 31, 32}. We start from the Lagrangian of the
spatially-discretized Vlasov-Maxwell system in Ref. [24],

\[ L_{sd} = \frac{1}{2} \left( \sum_j \left( -\dot{A}_J - \sum_I \nabla_{d,I} \phi_I \right)^2 - \sum_K \left( \sum_J \text{curl}_{d,K,J} A_J \right)^2 \right) \Delta V + \]
\[ \sum_s \left( \frac{1}{2} m_s \dot{x}_s^2 + q_s \left( \dot{x}_s \cdot \sum_J W_{\sigma_{1,J}} (x_s) A_J - \sum_I W_{\sigma_{0,I}} (x_s) \phi_I \right) \right) . \] (7)

Here, integers \( I, J \) and \( K \) are indices of grid points in a cubic-mesh, and \( \nabla_d, \text{curl}_d \) and \( \text{div}_d \) are the discrete gradient, curl and divergence operators defined as follows,

\[
(\nabla_d \phi)_{i,j,k} = [\phi_{i+1,j,k} - \phi_{i,j,k}, \phi_{i,j+1,k} - \phi_{i,j,k}, \phi_{i,j,k+1} - \phi_{i,j,k}] ,
\] (8)

\[
(\text{curl}_d A)_{i,j,k} = 
\begin{bmatrix}
A_{z,i,j,k+1} - A_{z,i,j,k} \\
A_{x,i,j,k+1} - A_{x,i,j,k} \\
A_{y,i,j+1,k} - A_{y,i,j,k} 
\end{bmatrix}^T ,
\] (9)

\[
(\text{div}_d B)_{i,j,k} = 
\begin{bmatrix}
B_{x,i+1,j,k} - B_{x,i,j,k} + B_{y,i,j+1,k} - B_{y,i,j,k} + B_{z,i,j+1,k} - B_{z,i,j,k} 
\end{bmatrix} .
\] (10)

These operators are local linear operators on the discrete fields \( \phi_I, A_J \) and \( B_K \). Functions \( W_{\sigma_{0,J}}, W_{\sigma_{1,J}} \) and \( W_{\sigma_{2,K}} \) are interpolation functions (Whitney forms) for 0-forms, e.g., scalar potential, 1-forms, e.g., vector potential, and 2-forms, e.g., magnetic fields, respectively.

These discrete operators and interpolation functions satisfy the following properties [24, 36, 38, 39],

\[
\nabla \sum_I W_{\sigma_{0,I}} (x) \phi_I = \sum_{I,J} W_{\sigma_{1,J}} (x) \nabla_{d,I} J \phi_I ,
\] (11)

\[
\nabla \times \sum_J W_{\sigma_{1,J}} (x) A_J = \sum_{J,K} W_{\sigma_{2,K}} (x) \text{curl}_{d,K,J} A_J ,
\] (12)

\[
\nabla \cdot \sum_K W_{\sigma_{2,K}} (x) B_K = \sum_{K,L} W_{\sigma_{3,L}} (x) \text{div}_{d,K,L} B_K .
\] (13)

Periodic boundary in all three directions are adopted to simplify the discussion. Because time \( t \) does not explicitly appear in the Lagrangian, the total energy

\[
H_{sd} = \frac{\partial L_{sd}}{\partial \dot{q}} \dot{q}^T - L_{sd}
\] (14)

\[
= \frac{1}{2} \Delta V \left( \sum_J E_J^2 + \sum_K B_K \right) + \sum_s \frac{1}{2} m_s \dot{x}_s^2
\] (15)

is conserved, i.e., \( \dot{H}_{sd} = 0 \). Here, \( q \) is the generalized coordinates, i.e., \( q = [A_J, \phi_I, x_s] \), and
\( E_J \) and \( B_K \) are discrete electromagnetic fields defined as
\[
E_J = -\dot{A}_J - \sum_j \nabla_{d,J} \phi_I, \quad (16)
\]
\[
B_K = \sum_j \text{curl}_{d,KJ} A_J. \quad (17)
\]
The corresponding Poisson bracket for this system is [24]
\[
\{ F, G \} = \frac{1}{\Delta V} \sum_j \left( \frac{\partial F}{\partial E_J} \cdot \sum_K \frac{\partial G}{\partial B_K} \text{curl}_{d,KJ} - \sum_K \frac{\partial F}{\partial B_K} \text{curl}_{d,KJ} \cdot \frac{\partial G}{\partial E_J} \right) + \\
\sum_s \frac{1}{m_s} \left( \frac{\partial F}{\partial x_s} \cdot \frac{\partial G}{\partial x_s} - \frac{\partial F}{\partial x_s} \cdot \frac{\partial G}{\partial \dot{x}_s} \right) + \\
\sum_s \frac{q_s}{m_s \Delta V} \left( \frac{\partial F}{\partial \dot{x}_s} \cdot \sum_j W_{\sigma_1J}(x_s) \frac{\partial G}{\partial E_J} - \frac{\partial G}{\partial \dot{x}_s} \cdot \sum_j W_{\sigma_1J}(x_s) \frac{\partial F}{\partial E_J} \right) + \\
- \sum_s \frac{q_s}{m_s^2} \frac{\partial F}{\partial \dot{x}_s} \cdot \left[ \sum_K W_{\sigma_2K}(x_s) B_K \right] \cdot \frac{\partial G}{\partial \dot{x}_s}. \quad (18)
\]

With this Poisson bracket, the time evolution of the system is
\[
\dot{g} = \{ g, H_{sd} \}, \quad (19)
\]
where \( g = [E_J, B_K, x_s, \dot{x}_s] \). Now we introduce the discrete local energy \( \epsilon_I \) at the \( I \)'th grid,
\[
\epsilon_I = \sum_s \frac{1}{2} m_s \dot{x}_s^2 W_{\sigma_0I}(x_s) + E_I^2 + B_I^2. \quad (20)
\]
The evolution of \( \epsilon_I \) is
\[
\dot{\epsilon}_I = \{ \epsilon_I, H_{sd} \}, \quad (21)
\]
or more specifically,
\[
\dot{\epsilon}_I = \sum_s q_s \left( \dot{x}_s \cdot \sum_{J'} E_{J'} W_{\sigma_1J'}(x_s) \right) W_{\sigma_0I}(x_s) + \sum_s \frac{1}{2} m_s \dot{x}_s^2 (x_s \cdot \nabla W_{\sigma_0I}(x_s)) + \\
E_I \cdot \sum_K \text{curl}_{d,KI} B_K - E_I \cdot \sum_s q_s \dot{x}_s W_{\sigma_1I}(x_s) - B_I \cdot \sum_j \text{curl}_{d,IJ} E_J. \quad (22)
\]

We will see that the right hand side of Eq. (22) can be written as a discrete divergence of a discrete vector field, which means that Eq. (22) is a discrete energy conservation law.

Let us divide the RHS of Eq. (22) into three terms,
\[
\dot{\epsilon}_I = T_1 + T_2 + T_3, \quad (23)
\]
where

\[ T_1 = E_I \cdot \sum_K \text{curl}_K B_K - B_I \cdot \sum_J \text{curl}_J E_J , \]  
\[ T_2 = \sum_s \frac{1}{2} m_s \dot{x}_s^2 (\dot{x}_s \cdot \nabla W_{\sigma_I} (x_s)) , \]  
\[ T_3 = \sum_s q_s \left( \dot{x}_s \cdot \sum_{J'} E_{J'} W_{\sigma_J J'} (x_s) \right) W_{\sigma_I} (x_s) - E_I \cdot \sum_s q_s \dot{x}_s W_{\sigma_I} (x_s) . \]  

Firstly, for \( T_1 \), we can check that this term can be written as a discrete divergence

\[ T_1 = - \sum_K \text{div}_K (E \times *B)_K , \]  

where \( E \times *B \) is defined as

\[
(E \times *B)_{i,j,k} = \begin{bmatrix}
E_{yi,j,k} B_{zi-1,j,k} - E_{zi,j,k} B_{yi-1,j,k} \\
E_{zi,j,k} B_{zi-1,j,k} - E_{xi,j,k} B_{zi-1,j,k} \\
E_{xi,j,k} B_{yi,j,k-1} - E_{yi,j,k} B_{zi,j,k-1}
\end{bmatrix}^T .
\]

Next, we investigate \( T_2 \) which represents the energy flow of particles,

\[ T_2 = \sum_s \frac{1}{2} m_s \dot{x}_s^2 (\dot{x}_s \cdot \nabla W_{\sigma_I} (x_s)) \]
\[ = \sum_s \frac{1}{2} m_s \dot{x}_s^2 \left( \dot{x}_s \cdot \sum_J W_{\sigma_J} (x_s) \nabla d_{JJ} \right) \]
\[ = \sum_J \nabla d_{JJ} \sum_s \frac{1}{2} m_s \dot{x}_s^2 \dot{x}_s \cdot W_{\sigma_J} (x_s) \]
\[ = \sum_J \nabla d_{JJ} S_J = - \sum_K \text{div}_K (*S)_K , \]  

where

\[ S_J = \sum_s \frac{1}{2} m_s \dot{x}_s^2 \dot{x}_s \cdot W_{\sigma_J} (x_s) , \]
\[ (*S)_K = [S_{xi-1,j,k}, S_{yi,j-1,k}, S_{zi,j,k-1}] . \]

Thus this term is also a discrete divergence. Finally, let us look at \( T_3 \), which appears only in the discrete particle-field system. It is

\[ T_3 = \sum_s q_s \left( \dot{x}_s \cdot \sum_{J'} E_{J'} W_{\sigma_J J'} (x_s) \right) W_{\sigma_I} (x_s) - E_I \cdot \sum_s q_s \dot{x}_s W_{\sigma_I} (x_s) \]
\[ = \sum_s q_s \left( \sum_{J'} \dot{x}_s \cdot E_{J'} W_{\sigma_J J'} (x_s) W_{\sigma_I} (x_s) - E_I \cdot \dot{x}_s W_{\sigma_I} (x_s) \right) \]
\[ = \sum_s q_s F (s) \left( W_{\sigma_I} (x_s) - \frac{p(s,I)}{F(s)} \right) , \]
where

\[ F(s) = \sum_I p(s, I) , \]  

\[ p(s, I) = E_I \cdot \dot{x}_s W_{\sigma I}(x_s) . \]  

From the definition of \( W_{\sigma I}(x) \), we have \( \sum_I W_{\sigma I}(x_s) = 1 \). Therefore,

\[ \sum_I \left( W_{\sigma I}(x_s) - \frac{p(s, I)}{F(s)} \right) = 0 , \]  

which means that the sum of \( T_3 \) over all spatial grid points vanishes. Now we invoke the two theorems approved in the Appendix, which states that a discrete sum-free field must be a discrete divergence field and that if the sum-free field is local, then the divergence field is local. Therefore, for each particle, \( T_3 \) can be expressed as discrete divergence of a discrete vector field \( G_s \),

\[ T_3 = \sum_s q_s \sum_{J'} \text{div}_{dJ'} G_{sJ'} F(s) . \]  

For a particular \( s \), \( W_{\sigma 0 I}(x_s) \), \( W_{\sigma 1 J}(x_s) \) are local near \( x_s \), so is \( W_{\sigma I}(x_s) - p(s, I) / F(s) \). Thus \( G_s \) is also local near \( x_s \).

Finally, we obtain the local energy conservation law for the spatial-discretized Vlasov-Maxwell system.

\[
\frac{\partial}{\partial t} \left( \sum_s \frac{1}{2} m_s \dot{x}_s^2 W_{\sigma I}(x_s) + E_I^2 + B_I^2 \right) + \\
\sum_K \text{div}_{dIK} \left( (E \times sB)_K + (sS)_K - \sum_s q_s G_{sk} F(s) \right) = 0 . \]  

In conclusion, we started from the Hamiltonian theory of the spatially-discretized Vlasov-Maxwell system, used the property of Whitney forms, and derived a discrete local energy conservation law. In practice the spatially-discretized Vlasov-Maxwell system also need a temporal discretize to become a numerical scheme, after which the total energy will not be an exact invariant. However if we apply a symplectic integrator to perform the temporal discretize, then the total energy error can be bounded within a small value for all simulation time-steps \[43, 46\]. Investigation on discrete conservation laws for such systems are planned for future work.
Appendix A: a discrete sum-free field is a discrete divergence field

In this appendix, we prove the following two theorems.

**Theorem 1.** If a discrete scalar field $R$ is sum-free, i.e.,

$$\sum_I R_I = 0 , \quad (A1)$$

then it can be expressed as a discrete divergence of a discrete vector field $G$, i.e.,

$$R_I = \sum_J \text{div}_d I J G_J . \quad (A2)$$

The discrete field $R$ in Theorem 1 can also be a function of the continuous spatial coordinate $x$, such as the Whitney form $W_{\sigma_0}(x)$. A discrete field or a field component $F(x)$ is called local, if for every $x_0$, there exists a positive constant $C$ such that

$$F_I(x_0) = 0 , \forall I \in \{ J \mid |x_J - x_0| > C \} . \quad (A3)$$

**Theorem 2.** If a discrete sum-free scalar field $R$ is local, then there exists a local discrete vector field $G$ such that Eq. (A2) holds.

These two theorems also imply that a (local) discrete sum-free vector field or tensor field can be expressed as a discrete divergence of a (local) tensor or high order tensor, because for each component of the vector field or tensor field, Theorems 1 and 2 apply. To prove these two theorems, we first prove the following three lemmas.

**Lemma 1.** The discrete scalar field $R_x(i', j', k')$ defined as

$$R_{xI}(i', j', k') = \begin{cases} 1, & \text{if } I = [i' + 1, j', k'] , \\ -1, & \text{if } I = [i', j', k'] , \\ 0, & \text{otherwise} , \end{cases} \quad (A4)$$

can be expressed as a composition of $\text{div}_d$ and a discrete vector field $G_x(i', j', k')$,

$$R_{xI}(i', j', k') = \sum_J \text{div}_d I J G_x(i', j', k') . \quad (A5)$$

**Proof.** Let $G_x(i', j', k')$ be

$$G_x(i', j', k') = \begin{cases} [-1, 0, 0], & \text{if } J = [i' + 1, j', k'] , \\ [0, 0, 0], & \text{otherwise} . \end{cases} \quad (A6)$$
Then it is straightforward to verify that
\[ R_{xI}(i', j', k') = \sum \text{div}_{I,J} \mathbf{G}_{xJ}(i', j', k') . \] (A7)

Using the similar technique, we can construct \( \mathbf{G}_y(i', j', k') \) and \( \mathbf{G}_z(i', j', k') \) for scalar fields \( R_y(i', j', k') \) and \( R_z(i', j', k') \) as well, i.e.,
\[
R_{yI}(i', j', k') = \begin{cases} 1, & \text{if } I = [i', j' + 1, k'] , \\ -1, & \text{if } I = [i', j', k'] , \\ 0, & \text{otherwise} , \\ \end{cases} \] (A8)
\[
R_{zI}(i', j', k') = \begin{cases} 1, & \text{if } I = [i', j', k' + 1] , \\ -1, & \text{if } I = [i', j', k'] , \\ 0, & \text{otherwise} , \\ \end{cases} \] (A9)
\[
\mathbf{G}_{yJ}(i', j', k') = \begin{cases} [0, -1, 0], & \text{if } J = [i', j' + 1, k'] , \\ [0, 0, 0], & \text{otherwise} , \\ \end{cases} \] (A10)
\[
\mathbf{G}_{zJ}(i', j', k') = \begin{cases} [0, 0, -1], & \text{if } J = [i', j', k' + 1] , \\ [0, 0, 0], & \text{otherwise} . \\ \end{cases} \] (A11)

\textbf{Lemma 2.} The discrete scalar field \( R^1(I_1, I_2) \) defined as
\[
R^1_{I}(I_1, I_2) = \begin{cases} -1, & \text{if } I = I_1 , \\ 1, & \text{if } I = I_2 , \\ 0, & \text{otherwise} \\ \end{cases} \] (A12)
can be written in the following form
\[
R^1_{I}(I_1, I_2) = \sum_{I' \in Y_x} a_x R_{xI}(I') + \sum_{I' \in Y_y} a_y R_{yI}(I') + \sum_{I' \in Y_z} a_z R_{zI}(I') , \] (A13)
where \( Y_x, Y_y \) and \( Y_z \) are some indices sets, and \( a_x, a_y \) and \( a_z \) are some integers.

\textbf{Proof.} Choose \( Y_x, Y_y \) and \( Y_z \) as
\[
Y_x = \{ [i, j, k] | \min(i_1, i_2) \leq i < \max(i_1, i_2), j = j_2, k = k_2 \} , \] (A14)
\[
Y_y = \{ [i, j, k] | i = i_1, \min(j_1, j_2) \leq j < \max(j_1, j_2), k = k_2 \} , \] (A15)
\[
Y_z = \{ [i, j, k] | i = i_1, j = j_1, \min(k_1, k_2) \leq k < \max(k_1, k_2) \} . \] (A16)
Choose $a_x$, $a_y$ and $a_z$ as

\[
\begin{align*}
a_x &= \begin{cases} 1, & \text{if } i_1 < i_2 \ , \\ -1, & \text{otherwise} \ , \end{cases} \quad (A17) \\
a_y &= \begin{cases} 1, & \text{if } j_1 < j_2 \ , \\ -1, & \text{otherwise} \ , \end{cases} \quad (A18) \\
a_z &= \begin{cases} 1, & \text{if } k_1 < k_2 \ , \\ -1, & \text{otherwise} \ . \end{cases} \quad (A19)
\end{align*}
\]

It is straightforward to verify that Eq. (A13) holds.

**Lemma 3.** A sum-free scalar field $R$ can be written as

\[
R_I = \sum_{[I',I''] \in Z} b_{[I',I'']} R_{I'}^\dagger (I',I'') \ , \quad (A20)
\]

where $Z$ is some index-pair set.

**Proof.** If $\forall I$ such that $R_I = 0$, then $Z$ can be chosen as $\emptyset$. Otherwise let $Y_d = \{I_1, I_2, I_3, \ldots\}$ is the index set such that if $I \in Y_d$, $R_I \neq 0$ and $I \notin Y_d$, $R_I = 0$. We can choose the index-pair set $Z$ as

\[
Z = \{[I',I'']| I' = I_1, I'' \in Y_d \text{ and } I'' \neq I_1\} , \quad (A21)
\]

where $I_1$ is one arbitrarily chosen element in $Y_d$, and the corresponding $b_{[I',I'']}$ is

\[
b_{[I',I'']} = R_{I''} . \quad (A22)
\]

Using the fact that

\[
R_{I_1} + \sum_{I'' \in Y_d \text{ and } I'' \neq I_1} R_{I''} = \sum_I R_I = 0 , \quad (A23)
\]

we have

\[
R_{I_1} = - \sum_{I'' \in Y_d \text{ and } I'' \neq I_1} R_{I''} . \quad (A24)
\]

Then it is straightforward to verify that Eq. (A20) holds.

Composing these three lemmas, we can see that the Theorems 1 and 2 are proved.
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