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Energy preservation and entropy in Lagrangian space- and time-staggered hydrodynamic schemes

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ABSTRACT

Usual space- and time-staggered (STS) "leap-frog" Lagrangian hydrodynamic schemes—such as von Neumann–Richtmyer's (1950), Wilkins' (1964), and their variants—are widely used for their simplicity and robustness despite their known lack of exact energy conservation. Since the seminal work of Trulio and Trigger (1950) and despite the later corrections of Burton (1991), it is generally accepted that these schemes cannot be modified to exactly conserve energy while retaining all of the following properties: STS stencil with velocities half-time centered with respect to positions, explicit second-order algorithm (locally implicit for internal energy), and definite positive kinetic energy.

It is shown here that it is actually possible to modify the usual STS hydrodynamic schemes in order to be exactly energy-preserving, regardless of the evenness of their time centering assumptions and retaining their simple algorithmic structure. Burton's conservative scheme (1991) is found as a special case of time centering which cancels the term here designated as "incompatible displacements residue." In contrast, von Neumann–Richtmyer's original centering can be preserved provided this residue is properly corrected. These two schemes are the only special cases able to capture isentropic flow with a third order entropy error, instead of second order in general.

The momentum equation is presently obtained by application of a variational principle to an action integral discretized in both space and time. The internal energy equation follows from the discrete conservation of total energy. Entropy production by artificial dissipation is obtained to second order by a prediction–correction step on the momentum equation.

The overall structure of the equations (explicit for momentum, locally implicit for internal energy) remains identical to that of usual STS "leap-frog" schemes, though complementary terms are required to correct the effects of time-step changes and artificial viscosity updates.

In deriving these schemes, an apparently novel approach of "flux-in-time" was introduced to correct numerical residues and ensure energy conservation. This method can be applied to essentially any numerical scheme whenever required or desired provided space and time numerical consistency is preserved.

Numerical test cases are presented confirming the conservative character of the new CSTS schemes down to computer round-off errors, and showing various improvements compared to the standard von Neumann–Richtmyer and Wilkins STS schemes, mostly on shock levels, shock velocities, singularity induced distortions, and CFL stability limits.

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Table 1
Kinetic energy definitions and properties of various space-staggered Lagrangian schemes from Trulio and Trigger [7], Burton [9], and as aimed at in the present work.

Ref.	Kinetic energy $(\boldsymbol{u}_p)^2$	Restrictions for exact energy conservation	Form of momentum equation
Trulio and Trigger [7]:			
Eq. 6b	$\frac{1}{2}\boldsymbol{u}_p^{n-1/2}\cdot\boldsymbol{u}_p^{n+1/2}$	Δt constant and $q=0$ (order 1 otherwise)	Explicit on $\boldsymbol{u}_p^{n-1/2}$ (VNR)
Eq. 6c	$\frac{1}{2}\boldsymbol{u}_p^{n-1/2}\cdot\boldsymbol{u}_p^{n+1/2}$	Δt constant (order 1 otherwise)	Explicit on $\boldsymbol{u}_p^{n-1/2}$ (implicit on q_c^{n+1})
Eq. E1	$\frac{1}{2}\boldsymbol{u}_p^{n-1/2}\cdot\boldsymbol{u}_p^{n+1/2}$	None	Explicit on $\boldsymbol{u}_p^{n}$
Eqs. R1–6	$\frac{1}{2}(\boldsymbol{u}_p^{n})^2$	None	Implicit on $\boldsymbol{u}_p^{n}$ (also [8, eq. 4.2.6])
Burton [9]:			
Eq. 5.2	$\frac{1}{2}\boldsymbol{u}_p^{n-1/2}\cdot\boldsymbol{u}_p^{n+1/2}$	Time centering of positions with respect to velocities, see Fig. 1c and (1)	Explicit on $\boldsymbol{u}_p^{n-1/2}$
& Eq. 5.4	$\frac{1}{2}(\boldsymbol{u}_p^{n-1/2})^2$		
Here:			
(7)	$\frac{1}{2}(\boldsymbol{u}_p^{n-1/2})^2$	None	Explicit on $\boldsymbol{u}_p^{n-1/2}$

1. Introduction

1.1. Present understanding of energy conservation in Lagrangian schemes

Over the nearly 70 years since the first practical calculations were carried out in weapons laboratories, the mathematical principles of numerical schemes for Computational Fluid Dynamics (CFD) have experienced very profound evolution: beyond the necessary adaptations to the staggering increase in computer power during this time, a major change has been a progressive drift away from the numerical options of the first schemes of von Neumann and Richtmyer [1–4]—here designated as "VNR."

The original VNR scheme [4] was designed as a simple finite differences Lagrangian algorithm—i.e. with an explicit momentum equation and a locally semi-implicit energy equation—which achieves second-order space-and-time accuracy through a "leap-frog" space-and-time staggering (STS) of variables. Although it exactly conserves mass and momentum, it conserves energy only to second order—first in the presence of shocks—and it may produce spurious transient oscillations as shock capture is achieved by adding artificial viscosity. Further developments extended the scheme in various directions (multiple dimensions [5,6], elastic–plastic behavior [5], Arbitrary Lagrange–Euler [6], etc.) but, *under the STS stencil constraint*, the lack of energy conservation had not received a satisfactory correction until the early 1990's. This was a major drawback in the presence of shocks, where correspondingly inaccurate Hugoniot jump conditions lead to zero order errors on their positions and magnitudes.

One decade after the VNR scheme was published, Trulio and Trigger provided the first 1D analysis of the energy non-conservation issue [7] with suggestions of modified schemes to regain it. Their conclusions are summarized in Table 1 where masses, velocities, and per mass kinetic energies are designated by m, $\boldsymbol{u}$, and $\boldsymbol{u}^2$, and labeled at nodes by p, and at integer and half-integer time steps by n and $n+1/2$. Since then, common wisdom has thus been that unconditional exact energy conservation—i.e. without restrictions on time step other than CFL—can only be achieved if velocity is centered at *integer labeled time instants* and if either: i) the (non-local) momentum equation is *implicit* in order for the kinetic energy to be a *positive definite* quadratic form of velocity, or ii) the kinetic energy is defined by a *non-positive* quadratic form of velocity in order for the momentum equation to be *explicit*.

However, in 1991 Burton revisited these findings—together with issues of nodal mass definition, variable time step, pressure gradient definition, and multiple dimensions—and provided *exact* energy conservation with an *explicit* momentum equation and a *positive definite* quadratic form for the kinetic energy [9, eqs. 4.6, 5.4 & 6.2] (see Table 1). This is achieved by considering the energy balance at *half-integer* labeled times, where kinetic energy is simply defined as squared velocity, but where internal energy must be inferred from its value at integer labeled times by correcting for pressure work over half time steps. However, when the time step is not constant, Burton's scheme requires the somewhat unusual centering of *positions* at times t^n with respect to *velocities* at times $t^{n+1/2}$—instead of the more intuitive centering of velocities with respect to positions—or

$$t^n=\tfrac{1}{2}(t^{n+1/2}+t^{n-1/2})\,,\quad \text{instead of}\quad t^{n+1/2}=\tfrac{1}{2}(t^{n+1}+t^{n})\,, \tag{1}$$

as shown in Fig. 1 below. In some cases, this may somewhat impact robustness and CFL limitations because now, *in contrast to the original STS scheme* the time step is estimated an extra half-time step earlier—for instance from the speed of sound c^n for time step δt^{n+1} instead of $\delta t^{n+1/2}$.

Puzzlingly, Burton's correction appears to have been little investigated, let alone included in CFD codes, despite its significant impact on shock accuracy and its marginal cost even when weighed by possibly minor defects. Yet, the extensive usage of the original VNR explicit scheme and its variants in non-conservative form persists to date, motivated by simplicity or legacy and notwithstanding the artifacts appearing for instance under strong shocks. At the same time, conservation