The Discrepancy Between Simulation and Observation of Electric Fields in Collisionless Shocks

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Recent time series observations of electric fields within collisionless shocks have shown that the fluctuating, electrostatic fields can be in excess of one hundred times that of the quasi-static electric fields. That is, the largest amplitude electric fields occur at high frequencies, not low. In contrast, many if not most kinetic simulations show the opposite, where the quasi-static electric fields dominate, unless they are specifically tailored to examine small-scale instabilities. Further, the shock ramp thickness is often observed to fall between the electron and ion scales while many simulations tend to produce ramp thicknesses at least at or above ion scales. This raises numerous questions about the role of small-scale instabilities and about the ability to directly compare simulations with observations.

Keywords: PIC simulation, electric field measurement, kinetic instabilities, collisionless shock, energy dissipation

1 INTRODUCTION

Collisionless shock waves are an ubiquitous phenomenon in heliospheric and astrophysical plasmas. They most often manifest as a nonlinearly steepened fast magnetosonic-whistler wave that has reached a stable balance between steepening and some form of irreversible energy dissipation. If a balance is reached, a stationary shock ramp is formed. The shock ramp is the part of shock transition region between upstream and downstream with an abrupt, discontinuity-like change in number density ($n_S$ where $s$ is the particle species), pressure1, quasi-static2 magnetic field magnitude vector ($B_o$), and bulk flow velocity ($V_{bulk}$). The thickness of this ramp is thought to depend upon macroscopic shock parameters like the fast mode Mach number ($M_f$), shock normal angle, $\theta_{Bn}$ (e.g., quasi-perpendicular shocks satisfy $\theta_{Bn} \geq 45^\circ$), and upstream averaged plasma beta (Sagdeev, 1966; Coroniti, 1970; Tidman & Krall, 1971; Galeev, 1976; Kennel et al., 1985).

The term collisionless derives from the fact that the shock ramp thickness ranges from several electron inertial lengths3 to an ion inertial length with the majority below $\sim 35 \lambda_e$ (Hobara et al., 2010; Mazelle et al., 2010). In contrast, the collisional mean free path of a thermal proton can be on the order of 1 AU or $\geq 10^7 \lambda_e$ (Wilson et al., 2018; Wilson et al., 2019a). Thus, fast mode shocks in astrophysical plasmas cannot be regulated by Coulomb collisions (with the exception of, perhaps,

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1$P_s = n_s k_B T_s$, where $T_s$ is the temperature of species $s$.

2Note we use the term quasi-static instead of background here since electromagnetic fluctuations near shocks in the solar wind can have amplitudes larger than the surrounding mean. That is, quasi-static refers to the lowest frequency response of an instrument, for practical purposes, but one can think of it as the effective background field.

3$\lambda = \frac{c}{\omega}$, where $s$ is the particle species.
TABLE 1 | Common Electrostatic Waves at/near Collisionless Shocks.

| Wave Name | Polarization or waveform | Frequency* and/or Appearance | Scale Length** | Free energy source or wave source |
|-----------|--------------------------|-------------------------------|----------------|----------------------------------|
| LHW       | linear \(\perp \) to \(\mathbf{B}_0\) or oblique to \(\mathbf{B}_0\) | \(f_{\text{lc}} \sim 5-40 \text{ Hz}\) \(f_{\text{lc}} \lesssim f_{\text{fl}}\) | \(k \lambda_e \lesssim 1\) | currents\(^4\), total charge, and incident electrons and incident ions. |
| IAW       | linear \(\parallel \) to \(\mathbf{B}_0\) or oblique to \(\mathbf{B}_0\) | \(f_{\text{lc}} \sim 10^{-2}-10^{6} \text{ Hz}\) \(f_{\text{na}} \lesssim \omega_{\text{ci}}\) symmetric modulated sine waves | \(\lambda \lesssim 2 \pi \lambda_{\text{De}}\) | relative drift between electron beams\(^5\) or nonlinear wave decay\(^5\). |
| ECDI      | elliptical or “Tear-drop”-shaped oblique to \(\mathbf{B}_0\) | \(f_{\text{lc}} \sim 10^{-2}-10^{6} \text{ Hz}\) \(f_{\text{na}} \sim \omega_{\text{ci}}\) asymmetric modulated sine waves | \(k \lambda_{\text{De}} \lesssim 1\) | nonlinear wave decay\(^5\). |
| ESW       | bipolar pulse \(\parallel \) to \(\mathbf{B}_0\) or \(\perp \) to \(\mathbf{B}_0\) | \(f_{\text{lc}} \sim 10^{-2}-10^{6} \text{ Hz}\) \(f_{\text{na}} \sim \omega_{\text{ci}}\) | \(\lambda \lesssim \lambda_{\text{De}}\) | electron beams\(^5\). |
| LW\(\gamma\) | linear \(\perp \) to \(\mathbf{B}_0\) or elliptical \(\perp \) to \(\mathbf{B}_0\) | \(f_{\text{lc}} \sim 10^{-2}-10^{6} \text{ Hz}\) | \(k \lambda_{\text{De}} \lesssim 1\) | electron beams\(^5\) and/or nonlinear wave decay\(^5\). |

*\(f_{\text{lc}}\) = spacecraft frame frequency; \(^{\text{t}}\)Wavelength or normalized wave number; \(^{\text{t}}\)free energy sources (e.g., initialize with two counter-streaming electron beams). Therefore, all of the modes listed in the following discussion have been generated in PIC simulations (Dyrud and Oppenheim, 2006; Matsukiyo and Scholer, 2006; Matsukiyo and Scholer, 2012; Muschietti and Lembège, 2017; Saito et al., 2017). However, as will be shown, parameters like the wavelengths and amplitudes tend to differ from those in observations, sometimes significantly.

Recent work using time series electric field data has shown that the common electrostatic wave modes near collisionless shocks include lower hybrid waves (LHWs), ion acoustic waves (IAWs), electrostatic solitary waves (ESWs), waves radiated by the electron cyclotron drift instability (ECDI), and Langmuir waves (Filbert and Kellogg, 1979; Mellott and Greenstadt, 1988; Kellogg, 2003; Wilson et al., 2007; Pulupa and Bale, 2008; Walker et al., 2008; Wilson et al., 2010; Breneman et al., 2013; Wilson et al., 2014a; Wilson et al., 2014b; Chen et al., 2018; Goodrich et al., 2018; Goodrich et al., 2019). The properties of these modes are summarized in Table 1 and discussed in detail below.

Electrostatic LHWs have been theorized to play a critical role in collisionless shock dynamics for decades (Papadopoulos, 1985; Tidman and Krall, 1971; Wu et al., 1984) but observations of their electrostatic form have been limited (Mellott and Greenstadt, 1988; Kellogg, 2003; Wilson et al., 2007; Pulupa and Bale, 2008; Walker et al., 2008; Wilson et al., 2010; Breneman et al., 2013; Wilson et al., 2014a; Wilson et al., 2014b; Chen et al., 2018; Goodrich et al., 2018; Goodrich et al., 2019). The properties of these modes are summarized in Table 1 and discussed in detail below.
Electrostatic IAWs have been observed in the solar wind and near collisionless shocks for over 40 years (Fredricks et al., 1968; Fredricks et al., 1970a; Gurnett and Anderson, 1977; Gurnett et al., 1979; Kurth et al., 1979). They present in spacecraft observations at frequencies, in the spacecraft frame, above the proton plasma frequency (due to the Doppler effect), typically in the ~1–10 kHz range in the solar wind near 1 AU. They are observed as linearly polarized (mostly parallel to \( B_0 \) but sometimes at small oblique angles), modulated sine waves with bursty wave envelopes lasting 10 s of ms (Wilson et al., 2007; Wilson et al., 2010; Wilson et al., 2014a; Wilson et al., 2014b). They have been shown to have wavelengths on the order of a few to several Debye lengths, or 10–100 s of meters near 1 AU (Fuselier and Gurnett, 1984; Breneman et al., 2013; Goodrich et al., 2018; Goodrich et al., 2019). They are thought to be driven unstable by the free energy in currents (Biskamp et al., 1972; Lemons and Gary, 1978), temperature gradients (Allan and Sanderson, 1974), electron heat flux (Dum et al., 1980; Henchen et al., 2019), or ion/ion streaming instabilities (Auer et al., 1971; Akimoto and Winske, 1985; Akimoto et al., 1985b; Goodrich et al., 2019) or they can result from a nonlinear wave-wave process (Cairns and Robinson, 1992; Dyrud and Oppenheim, 2006; Kellogg et al., 2013; Saito et al., 2017). These modes are important for collisionless shock dynamics because they can stochastically accelerate thermal electrons (parallel to \( B_0 \)) generating self-similar velocity distribution functions (VDFs) or the so-called “flattop” distributions (Vedenov, 1963; Sagdeev, 1966; Dum et al., 1974; Dum, 1975; Dyrud and Oppenheim, 2006). They are also capable of stochastically accelerating the high energy tail of the ion VDF (parallel to \( B_0 \)) (Dum et al., 1974). Note that the generation of the flattop has recently been interpreted as evidence of inelastic collisions (Wilson et al., 2019a; Wilson et al., 2019b; Wilson et al., 2020).

ESWs present in spacecraft observations as short duration (few ms), bipolar electric field pulses parallel to \( B_0 \) and monopolar perpendicular (Behlke et al., 2004; Wilson et al., 2007; Wilson et al., 2010; Wilson et al., 2014b). They tend to be on Debye scales and are thought to be BGK phase space holes (Ergun et al., 1998; Cattell et al., 2005; Franz et al., 2005; Vasko et al., 2018). ESWs can be driven unstable by electron beams (Ergun et al., 1998; Cattell et al., 2005; Franz et al., 2005), ion beams (Vasko et al., 2018), modified two-stream instability (MTSI) (Matsukiyo and Scholer, 2006), or the produce of high frequency wave decay (Singh et al., 2000). Until recently, it was thought all ESWs outside the auroral acceleration region were electron holes. However, work by (Vasko et al., 2018) and (Wang et al., 2020) suggest that many of the ESWs in the terrestrial bow shock are not only ion holes, they do not propagate exactly along \( B_0 \) as was previously thought. ESWs are important in collisionless shock dynamics because they can trap incident electrons (Dyrud and Oppenheim, 2006; Lu et al., 2008) or ions (Vasko et al., 2018; Wang et al., 2020), depending on the type of hole. They have also been shown to dramatically heat ions (Ergun et al., 1998), and/or couple to (or directly cause) the growth of IAWs (Dyrud and Oppenheim, 2006), whistler mode waves (Singh et al., 2001; Lu et al., 2008; Goldman et al., 2014), LHWs (Singh et al., 2000).

The ECDI is driven by the free energy in the relative drift between the incident electrons and shock-reflected ions (Forslund et al., 1970; Forslund et al., 1971; Lampe et al., 1972; Matsukiyo and Scholer, 2006; Muschietti and Lembège, 2013). They also range from Debye to electron thermal gyroradius scales (Breneman et al., 2013) and present in spacecraft observations as mixtures of Doppler-shifted IAWs and electron Bernstein modes. The polarization of these modes can be confusing, presenting as shaped like a tadpole or tear drop, with one part of the “tadpole” nearly parallel to \( B_0 \), and the other nearly orthogonal (i.e., the Bernstein mode part) (Wilson et al., 2010; Breneman et al., 2013; Wilson et al., 2014b; Goodrich et al., 2018). This results from the coupling between two modes that are normally orthogonal to each other in their electric field oscillations. ECDI-driven modes are important for collisionless shocks because they can resonantly interact with the bulk of the ion VDF, generate a suprathermal tail on the ion VDF, and strongly heat the electrons perpendicular to \( B_0 \) (Forslund et al., 1970; Forslund et al., 1972; Lampe et al., 1972; Muschietti and Lembège, 2013).

Langmuir waves have been observed upstream of collisionless shocks for decades (Gurnett and Anderson, 1977; Felbert and Kellogg, 1979; Kellogg et al., 1992; Cairns, 1994; Bale et al., 1998; Bale et al., 1999; Malaspina et al., 2009; Soucek et al., 2009; Krasnoselskikh et al., 2011). These waves have \( k \lambda \approx 1 \) (Soucek et al., 2009; Krasnoselskikh et al., 2011) and rest frame frequencies satisfying \( f_{freq} \leq f_{pe} \). Langmuir waves are driven unstable by electron beams and/or nonlinear wave decay (Pulupa et al., 2010; Kellogg et al., 2013). They tend to be linearly polarized nearly parallel to \( B_0 \) when electrostatic but some do exhibit circular polarization when electromagnetic (Bale et al., 1998; Malaspina and Ergun, 2008). Langmuir waves are relevant to collisionless shock dynamics in that they dissipate the free energy in reflected electron beams and can mode convert to generate free mode emissions that can serve as remote detection signatures (Cairns, 1994; Bale et al., 1999; Pulupa et al., 2010).

In summary, the most commonly observed electrostatic wave modes near collisionless shocks are IAWs, ESWs, ECDI-driven modes, and Langmuir waves. Electrostatic LHWs are less commonly observed, which may be due to instrumental effects.

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\( n_e = \sqrt{\frac{2e}{\pi \epsilon_0 3k T_e}} \) where \( n_e \) is the electron number density.

\( f_{pe} = \sqrt{\frac{2e T_e}{m_e}} \) where \( f_{pe} \) is the electron plasma frequency.
as many electric field instruments (Bonnell et al., 2008; Bougeret et al., 2008; Cully et al., 2008) have been designed with gain roll-offs at \( \sim 10 \) Hz (low- or high-pass filters), which happens to be the typical value of \( f_{\text{pe}} \) in the solar wind near 1 AU. It may also be that electrostatic LHWs are just less commonly generated or damp very quickly in collisionless shocks. Langmuir waves tend to occur upstream of the shock in regions filled with shock reflected electron beams (Cairns, 1994; Bale et al., 1999; Wilson et al., 2007; Pulupa et al., 2010). Although they can be common in the upstream, they tend to be much less so in the ramp and immediate downstream region. Therefore, the remaining discussion will focus on the most commonly observed Debye-scale, electrostatic modes: IAWs, ESWs, and ECDI-driven modes. These three modes are observed in and around both quasi-parallel and quasi-perpendicular shocks. The only macroscopic shock parameters on which they appear to depend are the shock density compression ratio and \( M_f \) [e.g., Wilson et al., 2007; Wilson et al., 2014a; Wilson et al., 2014b]. The ECDI-driven modes tend not to be observed for \( M_f \lesssim 3 \), since they require sufficient reflected ions to initiate the instability. Part of the reason for the lack of dependence on shock geometry is that the fluctuations in the foreshock upstream of a quasi-parallel shock, for instance, locally rotate the magnetic field to quasi-perpendicular geometries and some can even locally reflect/energize particles [e.g., Wilson et al., 2013; Wilson et al., 2016].

2 HISTORICAL CONTEXT

2.1 Spacecraft Observations

Early spacecraft electric field observers had very limited resources, compared to modern day, in memory, computational power, and spacecraft telemetry. As such, the common practice was to perform onboard computations to generate Fourier spectra for predefined frequency ranges (Fredricks et al., 1968; Fredricks et al., 1970a; Fredricks et al., 1970b; Rodriguez and Garnett, 1975). These Fourier spectra are spectral intensity data averaged over fixed time and frequency intervals, which has been more recently shown to significantly underestimate the instantaneous wave amplitude (Tsurutani et al., 2009). The underestimation led to some confusion in multiple areas of research because the estimated wave amplitudes from the spectra were too small to noticeably impact the dynamics of the system in question.

For instance, for decades the radiation belt community had relied upon such dynamic spectra and came to conclusion that the whistler mode waves (e.g., chorus and hiss) were typically in the \( \lesssim 1 \) mV/m amplitude range. The advent of time series electric field data led to the discovery that some of these modes could have amplitudes in excess of \( \sim 30 \) mV/m (Santolik et al., 2003). Later the STEREO spacecraft were launched and the electric field instruments were one of the first to be turned on. This led to the discovery of extremely large amplitude whistler mode waves with \( \gtrsim 200 \) mV/m (Cattell et al., 2008). The discovery provoked an investigation of \textit{Wind} observations as it passed through the radiation belt some 60+ times early in its lifetime. The result was a series of papers using \textit{Wind} and STEREO that all showed consistent observations of large amplitude whistler mode waves with \( \gtrsim 100 \) mV/m (Kellogg et al., 2010; Breneman et al., 2011; Kellogg et al., 2011; Kersten et al., 2011; Wilson et al., 2011; Breneman et al., 2012). These results altered the design and scientific direction of NASA’s \textit{Van Allen Probes} mission.

Similar issues arose in observations of collisionless shock waves. The early work using dynamic spectra data found electrostatic waves with spacecraft frame frequencies, \( f_{\text{se}} \), greater than a few hundred hertz to have amplitudes of, at most, a few 10s of mV/m but typically smaller in the few mV/m range (Fredricks et al., 1970b; Rodriguez and Garnett, 1975). Numerous theoretical studies had suggested that small-scale, high frequency waves were an important dissipation mechanism to regulate the nonlinear steepening of collisionless shock waves (Sagdeev, 1966; Tiead and Krall, 1971; Papadopoulos, 1985). However, such small amplitude electric field observations raised doubts about the ability of the high frequency modes to supply sufficient dissipation to maintain a stable shock.

The first published example (of which the authors are aware) of a time series electric field component observed by a spacecraft within a collisionless shock was presented in Wygant et al. (1987) observed by the ISEE-1 probe. The observation was one of the first pieces of evidence that the dynamic spectra plots were not fully capturing the electric field dynamics because the data showed electric fields up to nearly \( \sim 100 \) mV/m. Later work using the \textit{Wind} spacecraft found ESWs in the terrestrial bow shock with amplitudes in excess of \( \sim 100 \) mV/m (Bale et al., 1998; Bale et al., 2002). A few bow shock crossings were observed with the \textit{Polar} spacecraft, which found nonlinear, electrostatic IAWs within the shock with amplitudes up to \( \sim 80 \) mV/m (Hull et al., 2006). The picture starting to emerge was that high frequency, electrostatic waves were common and large amplitude in collisionless shocks. Note that the occurrence rate of electrostatic waves was already implied by studies using dynamic spectra data, but not such large amplitude.

Wilson et al. (2007) examined waveform capture data of electrostatic waves above the proton cyclotron frequency, \( f_{\text{pp}} \), from the \textit{Wind} spacecraft finding a positive correlation between peak wave amplitude and shock strength, i.e., stronger shocks had larger amplitude waves. They also observed that ion acoustic waves were the dominant electrostatic mode within the shock ramp. Shortly after, a study (Wilson et al., 2010) of a supercritical shock showed evidence of waves radiated by the ECDI. Since then, a series of papers using MMS (Chen et al., 2018; Goodrich et al., 2018; Goodrich et al., 2019), STEREO (Breneman et al., 2013), THEMIS (Wilson et al., 2014a; Wilson et al., 2014b), and \textit{Wind} (Breneman et al., 2013) have examined these electrostatic waves in collisionless shocks.

While the discussion has almost exclusively focused on fluctuating electric fields, \( \delta E \), it is critical to discuss quasi-static electric fields, \( E_o \), as well. The primary obstacle to accurate \( E_o \) measurements results from the lack of a stable ground in spacecraft observations (Scime et al., 1994a; Scime et al., 1994b; Scudder et al., 2000; Pulupa et al., 2014; Lavraud and Larson, 2016) and the sheath that forms around the conducting surfaces (Ergun et al., 2010), which alters how the instrument
couples to the plasma. It is beyond the scope of this study to
discuss, in detail, the difficulties associated with such
measurements, but some context can be gained by reviewing
some recent electric field instrument papers (Wygant et al., 2013;
Bale et al., 2016; Ergun et al., 2016; Lindqvist et al., 2016). In lieu
of a proper \( E_o \) measurement in the plasma rest frame, we
can estimate the convective electric field, \( E_c = -V_{sw} \times B_o \) (where \( V_{sw} \) is
the bulk flow solar wind velocity in the spacecraft frame)\(^8\). Since
the parameters in most simulations are scaled or normalized, we
will use the dimensionless ratio \( \delta E/E_o \) when comparing spacecraft
and simulation results. Unless otherwise specified, \( E_r = E_o \) in these
contexts.

Prior to the launch of MMS, there were several studies that
attempted to measure the cross shock electric field but each
suffered from inaccuracies or under resolved electric field
measurements which kept the issue of its magnitude in doubt
(Dimmock et al., 2011; Dimmock et al., 2012; Wilson et al., 2014a;
Wilson et al., 2014b). The launch of MMS allowed researchers, for
the first time, to probe \( E_o \) with sufficient cadence and accuracy to
properly measure the cross shock electric field in an
interplanetary shock (Cohen et al., 2019). Note that the \( E_o \)
measured in this study peaked at \( \leq 1.5 \) mV/m, i.e., comparable
to or smaller than the magnitude of \( E_c \) (which was \( \leq 4 \) mV/m
in this study). Therefore, we will assume \( E_o \) as being comparable to
\( E_c \) in magnitude throughout and will just refer to \( E_o \) instead of
both. Even so, there is some discrepancy because such a
measurement is extremely difficult at the terrestrial bow shock
and detailed MMS observations showed that the electron
dynamics seemed to be dominated by a combination of
magnetosonic-whistler modes and electrostatic IAWs and
ECDI waves (Chen et al., 2018).

The current picture from observations is summarized in the
following. In the studies where the quasi-static electric field could
be reliably measured (Cohen et al., 2019) or approximated from
measurements (Wilson et al., 2014a; Wilson et al., 2014b;
Goodrich et al., 2018; Goodrich et al., 2019), the findings were
that \( \delta E \) is consistently much larger than \( E_o \), i.e., \( \delta E \gg E_o \). Some of
these works attempted to quantify the impact on the dynamics of
the system due to \( \delta E \) vs. \( E_o \), finding \( \delta E \) dominated (Wilson et al.,
2014a; Wilson et al., 2014b; Chen et al., 2018; Goodrich et al.,
2018). Chen et al. (Chen et al., 2018) examined in great detail
the evolution of the electron distribution through the shock finding
that a magnetosonic-whistler wave accelerated the bulk of the
incident distribution which rapidly became unstable to high
frequency, electrostatic IAWs that scattered the electrons into
the often observed flattop distribution [Wilson et al., 2019b;
Wilson et al., 2019a; Wilson et al., 2020, and references therein]. This seems to somewhat
contradict the results of Cohen et al. (2019) and others who argued
that a quasi-static cross shock potential is dominating the shock and particle
dynamics. What all of these studies do agree upon is that
\( \delta E \gg E_o \). Note that the purpose of comparing the fluctuating
to the quasi-static field here is to help compare with simulations,
which normalize the electric fields by the upstream \( E_o \) value or
something similar.

**Figure 1** shows seven waveform captures observed by the
*Wind* spacecraft’s WAVES instrument (Bougeret et al., 1995)
while passing through the quasi-perpendicular terrestrial bow
shock. The first column shows the \( x \)-antenna electric field (\( \delta E_x \)),
the second the \( y \)-antenna electric field (\( \delta E_y \)), and the third
hodograms of \( \delta E_x \) vs. \( \delta E_y \). The local \( B_0 \) is projected onto
each hodogram shown as a magenta line\(^9\). Each row shows a different
waveform capture/snapshot that is \( \sim 17 \) ms in duration. The first
column contains a double-ended arrow in each panel illustrating
the scale associated with 200 mV/m. The first two rows show
examples of ESWs mixed with ECDI-driven waves, the third
and fourth rows show ECDI-driven waves, and the fifth through
seventh rows show IAWs. The distinguishing features are as
follows: the ESWs have an isolated, bipolar pulse with either a
linear or figure eight-like polarization and a nearly flat frequency
(spacecraft frame) spectrum response in the \( \sim 0.2-10 \) kHz range
(not shown); the IAWs exhibit symmetric \( \delta E_x \) and \( \delta E_y \) about zero,
are linearly polarized along \( B_o \) and have a broad frequency
peak (spacecraft frame) in the \( \sim 2-10 \) kHz range (not shown); and
the ECDI exhibit asymmetric \( \delta E_x \) and \( \delta E_y \), fluctuations about
zero, their polarization is not always linear along \( B_o \), and the
frequency peak (spacecraft frame) is in the \( \sim 0.5-10 \) kHz range
with superposed cyclotron harmonics (not shown). For reference,
the upstream average convective for this bow shock crossing is
\( E_o \sim 3.5 \) mV/m.

### 2.2 Kinetic Simulations

Kinetic simulations of shocks are challenging due to the need to
resolve global structure of the shock (generally associated with
\( \lambda_i \)\(^{10} \)) and the relatively long time scales associated with it
simultaneously with short spatial (\( \lambda_{De} \) and fast temporal
scales (\( f_i \)) associated with instabilities.

Early kinetic particle-in-cell (PIC) simulations were much
more limited by computational constraints than those
performed today. A common approach to scaling the problem
in order reduce the computational load is to consider one- or two-
dimensional problems and to reduce ratios of the ion-to-electron
mass, \( m_i/m_e \) and electron plasma-to-cyclotron frequency, \( \omega_{pe}/\omega_{ci} \),
while keeping the plasma \( \beta \) and the size of the problem in units of \( \lambda_i \)
comparable to the physical system of interest. Further
computational trade-offs include altering the simulation
resolution (i.e., number of grid cells), the number of particles
per cell for particle codes or velocity-space resolution for continuum
Vlasov codes (Yang et al., 2013). Since the frequencies and the growth rates of the instabilities of interest
are associated with certain characteristic time scales, such a re-
scaling may significantly alter the development and the role
of instabilities in the simulations. For example, reducing \( m_i/m_e \) lowers
the threshold for Buneman instability (Hoshino and Shimada,

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\(^8\)Note that the data is taken in the ecliptic plane to within \( \sim 1^\circ \) and the fraction of the
local \( B_0 \) in this plane exceeds 89% for all events except the first two rows.

\(^9\)The size of the problem may significantly exceed \( \lambda_i \), for example when upstream
turbulence in quasi-parallel shocks must be included.
by reducing the difference between electron and ion thermal speeds. Values of $\frac{\omega_{pe}}{\Omega_{ce}}$ were also expected and found to inhibit the growth of certain wave modes like Bernstein modes (Matsukiyo and Scholer, 2006; Muschietti and Lembège, 2013; Muschietti and Lembège, 2017). What’s more, the $\frac{M_i}{M_e}$ ratio was shown to dramatically affect the macroscopic profile of the shock magnetic field (Scholer and Matsukiyo, 2004) and affect the growth of what are now viewed as critical instabilities like the MTSI (Umeda et al., 2012a; Umeda et al., 2012b; Umeda et al., 2014). Thus the re-scaling approach must be carefully chosen based upon its expected impact on the phenomena of interest.

Some of the first two-dimensional PIC simulations using realistic $\frac{M_i}{M_e}$ was presented by (Matsukiyo and Scholer, 2006). Since then, the community has made efforts to compromise somewhat on $\frac{M_i}{M_e}$ in order to increase $\frac{\omega_{pe}}{\Omega_{ce}}$, to more realistic values (i.e., 50–100 in solar wind near 1 AU) (Muschietti and Lembège, 2013) used ratios of $\frac{M_i}{M_e} = 400$ and $\frac{\omega_{pe}}{\Omega_{ce}} = 10$ to examine the higher harmonics of Bernstein modes associated with the ECDI. More typical values for the latter fall in the $\sim 2–4$ range for recent simulations (Umeda et al., 2014; Matsukiyo and Matsumoto, 2015; Zeković, 2019). However, much larger values have been used in cases where one can reduce the simulation to one spatial dimension (Umeda et al., 2019).

Despite all of the progress made since the early full PIC simulations, there still remains two striking discrepancies between observations and many simulations: the amplitude and wavelength at which the strongest electric fields are observed and inconsistencies in the thickness of the shock ramp. The second issue is more obvious from cursory examinations of simulation results, so we will discuss it first.

As previously discussed, observations consistently show that the shock ramp thickness, $L_{sh}$, tends to satisfy $5 < L_{sh}/\lambda_e < 40$ (Hobara et al., 2010; Mazelle et al., 2010). However, PIC simulations, even with realistic mass ratio, often generate
shock ramps with thicknesses satisfying $L_{sh}/\lambda_c > 43$, i.e., exceeding proton inertial length (Scholer and Burgess, 2006), while some generate more realistically thin ramps (Matsukiyo and Scholer, 2012; Yang et al., 2013). Yang et al. (Yang et al., 2013) concluded that the shock ramp thickness decreased with increasing $\alpha_e/\lambda_c$ but increased with increasing ion plasma beta. Note however that (Matsukiyo & Scholer, 2012) used ~20% finer grid resolution, twice as many particles per cell, and smaller plasma betas than (Scholer & Burgess, 2006). However, (Yang et al., 2013) used fewer particles per cell and smaller $\alpha_e/\lambda_c$ than both (Matsukiyo and Scholer, 2012) and (Scholer and Burgess, 2006). It is important to note that it’s still not clear what physical or numerical parameters controls the ramp thickness in simulations or observations or even what the relevant physical scale is (e.g. $\lambda_e$ or $\lambda_D$).

Note that the thickness of the magnetic ramp of a collisionless shock is not significantly affected by the presence of corrugation/ripples (Johlander et al., 2016) other than the temporal dependence that can occur during reformation (Mazelle et al., 2010). The spatial extent of the entire transition region can indeed be increased by such oscillations but the magnetic gradient scale length does not appear to be significantly affected. The biggest limitation to determining the shock ramp thickness in data is time resolution. More recent spacecraft like THEMIS (Angelopoulos, 2008) and MMS (Burch et al., 2016) have, for instance, fluxgate magnetometers that return 3-vector components 128 times every second, which is more than sufficient to resolve the bow shock ramp. The bow shock moves slower in the spacecraft frame than interplanetary shocks, so time resolution is more of a constraint for examining the shock ramp thickness of interplanetary shocks. Even so, the 128 sps of the THEMIS and MMS fluxgate magnetometers is still sufficient for most interplanetary shocks.

As previously discussed, observations consistently show $\delta E/E_o > 50$ for fluctuations with wavelengths at or below a few 10s of Debye lengths (Wilson et al., 2014a; Wilson et al., 2014b; Chen et al., 2018; Goodrich et al., 2018), i.e, $\lambda \leq$ few 10s of $\lambda_{De}$. Most shock simulations find values satisfying $\delta E/E_i < 10$ and the scales at which the largest electric field fluctuations occur tend to satisfy $k\lambda_c < 1$ (Scholer and Matsukiyo, 2004; Matsukiyo and Scholer, 2006; Scholer and Burgess, 2007; Lembègue et al., 2009; Umeda et al., 2012a; Umeda et al., 2014; Matsukiyo and Matsumoto, 2015). We note that explicitly kinetic PIC simulations tend to have spatial grid resolution of a few $\lambda_{De}$, since such scales must be resolved for numerical stability. It has long been known that unrealistically small values of $\frac{\Delta x}{\lambda_{De}}$ and $\frac{\Delta t}{\Omega_{ce}}$ can lead to unrealistically large electric field amplitudes for modes with $k\lambda_c < 1$ (Hoshino and Shimada, 2002; Comisöl et al., 2011; Zeković, 2019). Although the three main modes discussed herein have been successfully identified in PIC simulations, they were either unrealistically small in amplitude or at different spatial scales or not excited unless the simulation was specifically tailored for that instability.

It is worth noting the severe computational costs of using fully realistic plasma parameters. The separation of spatial scales satisfies $\lambda_i/\lambda_{De} = \sqrt{\frac{m_i}{m_e}} P_i^{-(\alpha_e/\lambda_c)}$ or $\lambda_i/\lambda_{De} = (\omega_{pe}/\Omega_{ce})^{(\alpha_e/\lambda_c)} = \frac{\Omega_{ce}}{\sqrt{\omega_{pe}/\Omega_{ce}}}$. Where $\omega_{pe} = \frac{B_z}{\sqrt{\mu_0 \pi \rho}} = \lambda_e \Omega_e$ and $\beta_c = \frac{4\eta_{ei} \mu_0 T_e}{B_z^2} = \left( \frac{V_T e}{\pi \rho \Omega_e} \right)^2$. If we use typical examples from 1 AU solar wind observations (see Section 3 for values) and let $\beta_c \sim 1$, then $\lambda_i/\lambda_{De} \sim 4,000–20,000$. The separation of temporal scales goes as $\left( \frac{\omega_{pe}}{\Omega_{ce}} \right)^{d_1} \left( \frac{M_i}{m_e} \right)^{d_{1/2}}$, where $d$ is the number of spatial dimensions used in the simulation. Thus, one can see that increasing $\left( \frac{\omega_{pe}}{\Omega_{ce}} \right)$ from ~10 to 100, even in a one-dimensional simulation, is at least 10 times more computationally expensive. It is also the case that simulations often use shock speeds satisfying $V_{Tp} < V_T e < U_{sh}$ while shocks in the solar wind tend to satisfy $V_{Tp} < U_{sh} \ll V_T e$ (see Section 3 for values and definitions). For explicit PIC codes, there are additional computational expenses since the time steps are tied to the grid cell size, which raises the order of both $\frac{\Delta x}{\lambda_{De}}$ and $\frac{\Delta t}{\Omega_{ce}}$ by one. Therefore, it can be seen that we are approaching a computational wall and it may require new classes of simulation codes to overcome these limitations if we hope to use fully realistic plasma parameters.

\[ \text{Note that } \omega_{pe}/\Omega_{ce} \text{ is larger by an additional factor of } \sqrt{M_i/m_e}. \]
3 EXAMPLE OBSERVATIONS VERSUS SIMULATIONS

In this section we will present two example observations made by the THEMIS (Angelopoulos, 2008) and MMS (Burch et al., 2016) missions to further illustrate the difference in magnitude between $\delta E$ and $E_o$. We will also present PIC simulation results with parameters representative of a wide class of simulations discussed in the literature. The purpose is to illustrate some limitations of simulations to provoke advancement in closing the gap between observations and simulations of collisionless shocks.

Figure 2 shows a direct comparison between $\delta E$ and $E_o$ observed by THEMIS-C during a terrestrial bow shock crossing adapted from Wilson III et al. (2014a) and Wilson III et al. (2014b). The study examined the energy dissipation rates estimated from $(J \cdot \delta E)$ (i.e., from Poynting’s theorem) due to the observed electric fields, $E$, and estimated current densities. They expanded $(J_o + \delta J) \cdot (E_o + \delta E)$ and found that $(J_o \cdot \delta E)$ was the dominant term, i.e., the fluctuating fields acted to limit the low frequency currents in/around the shock. Two important things were found: the magnitude of $(J_o \cdot \delta E)$ and changes in this term were much larger than $(J_o \cdot E_o)$; the signs of the changes in $(J_o \cdot \delta E)$ and $(J_o \cdot E_o)$ are opposite. The second point was interpreted to imply that the fluctuating fields were giving energy to the particles and the quasi-static fields were gaining energy from the particles. In short, the main conclusion from Wilson III et al. (2014a; Wilson III et al., 2014b) was to illustrate that not only are the fluctuating electric fields large, they could potentially contribute enough energy transfer to compete with quasi-static fields. Prior to this study, the view by many in the community was that these fluctuating fields were completely negligible or just a minor, secondary effect. More recent, independent studies have performed similar analyses using different spacecraft and came to similar conclusions (Chen et al., 2018; Goodrich et al., 2018; Hull et al., 2020).

Figure 3 provides another example directly comparing $\delta E$ and $E_o$ observed by two MMS spacecraft during a terrestrial bow shock crossing. The electric fields are shown in the De-spun, Sun-pointing, L-vector system or DSL (Angelopoulos, 2008). For each spacecraft, $E_{adj} \leq 10$ mV/m was satisfied for the entire interval with most time steps satisfying $E_{adj} \leq 5$ mV/m. In contrast, the peak-to-peak $\delta E_j$ values commonly exceed 100 mV/m in bursty, short duration, wave packet intervals. Note that even the electric field instrument on MMS has limitations in its accuracy for frequencies below ~1 Hz (Ergun et al., 2016; Lindqvist et al., 2016). Thus, even with the significantly improved instrument technology and design of MMS, the observations consistently show $\delta E > E_o$.

As a practical list of reference values, we present one-variable statistics of solar wind parameters from the same data set as in Wilson et al. (2018) and all interplanetary (IP) shocks in the Harvard

Smithsonian’s Center for Astrophysics Wind shock database. The following will show parameters as $X_{50\%} \leq \bar{X} \leq X_{95\%}$, $\bar{X}$ [units], for the entire data set, where $X_{p\%}$ is the $p\%$ percentile and $\bar{X}$ is the median. First, the typical parameters for over 400 IP shocks are as follows:

\[
\begin{align*}
1.10 & \leq M_f \leq 4.60, \sim 1.91 \text{ [N/A]}; \\
1.15 & \leq M_A \leq 6.24, \sim 2.41 \text{ [N/A]}; \\
36.6 & \leq U_{shn} \leq 329.9, \sim 98.2 \text{ [km/s]}; \\
79.6 & \leq V_{shn} \leq 762.3, \sim 418.5 \text{ [km/s]}; \\
22.2 & \leq \theta_{fin} \leq 87.7, \sim 63.8 \text{ [deg]}; \\
\end{align*}
\]

Note that similar current densities have been found using multi-spacecraft techniques (Hull et al., 2020) supporting the results in Wilson III et al. (2014a) and Wilson III et al. (2014b).

Note that $Q^*$ in this context is not the quasi-static terms in quasi-linear or linear theory but that from the DC-coupled measurements. Further, $\delta Q$ is the fluctuating terms from these theories but the AC-coupled measurements, thus there is no a priori requirement that $\delta Q = 0$.

Footnotes:
12Note that similar current densities have been found using multi-spacecraft techniques (Hull et al., 2020) supporting the results in Wilson III et al. (2014a) and Wilson III et al. (2014b).
13Note that $Q^*$ in this context is not the quasi-static terms in quasi-linear or linear theory but that from the DC-coupled measurements. Further, $\delta Q$ is the fluctuating terms from these theories but the AC-coupled measurements, thus there is no a priori requirement that $\delta Q = 0$.
14https://www.cfa.harvard.edu/shocks/wi_data/.
where $U_{shn}$ is the upstream average flow speed in the shock rest frame and $V_{shn}$ is the upstream average shock speed in the spacecraft frame. Note that the values of $M_f$, $M_A$, and $U_{shn}$ will all be, on average, larger for most bow shocks in the interplanetary medium. These values are only meant to serve as a statistical baseline for reference. For example, the 11 bow shock crossings in Wilson et al. (2014a); Wilson et al. (2014b) satisfied $3.1 \leq M_A \leq 21.9$. Next, we present some typical plasma parameters near 1 AU in the solar wind:

$80.2 \leq f_{ce} \leq 409$, $\sim 162$ [Hz];

$0.04 \leq f_{fp} \leq 0.22$, $\sim 0.09$ [Hz];

$17.2 \leq f_{pe} \leq 42.5$, $\sim 26.3$ [kHz];

$371 \leq f_{ps} \leq 944$, $\sim 578$ [Hz];

$1.579 \leq V_{Te} \leq 2.411$, $\sim 1.975$ [km/s];

$21.9 \leq V_{Tp} \leq 76.9$, $\sim 40.2$ [km/s];

$1.03 \leq \rho_{ce} \leq 4.62$, $\sim 2.28$ [km];

$32.5 \leq \rho_{cp} \leq 186$, $\sim 88.8$ [km];

$1.12 \leq \lambda_e \leq 2.77$, $\sim 1.82$ [km];

$50.5 \leq \lambda_p \leq 129$, $\sim 82.5$ [km];

$4.74 \leq \lambda_{De} \leq 13.8$, $\sim 8.58$ [m];

where $f_{cs}$ is the cyclotron frequency of species $s$, $f_{ps}$ is the plasma frequency of species $s$, $V_{Te}$ is the most probable thermal speed of species $s$, $f_{fp}$ is the plasma frequency of species $s$, $\rho_{cs}$ is the thermal gyroradius of species $s$, and $\lambda_{De}$ is the electron Debye length.

$\frac{1}{\kappa} = \sqrt{\frac{T_e}{m_e}}$

$\frac{1}{\kappa} = \sqrt{\frac{T_e}{m_e}}$
Next, we present ratios of some typical plasma parameters near 1 AU in the solar wind:

\[
176 \leq \lambda_e/\lambda_{De} \leq 269, \sim 215 \text{ [NIA]};
\]
\[
131 \leq \rho_i/\lambda_{De} \leq 670, \sim 255 \text{ [NIA]};
\]
\[
8,000 \leq \lambda_e/\lambda_{De} \leq 12,160, -9.757 \text{ [NIA]};
\]
\[
0.34 \leq \lambda_c/\lambda_{De} \leq 1.63, -0.83 \text{ [NIA]};
\]
\[
92.4 \leq f_{pe}/f_{ce} \leq 474, \sim 180 \text{ [N/A]};
\]
\[
4.79 \leq V_i/\langle U_{shn}\rangle_{yx} \leq 7.31, -5.99 \text{ [NIA]};
\]
\[
43.1 \leq V_i/\langle U_{shn}\rangle_{yx} \leq 65.9, \sim 54.0 \text{ [NIA]};
\]
\[
0.53 \leq V_i/c \leq 0.80, \sim 0.66 \text{ [%]};
\]

where \(\langle U_{shn}\rangle_{yx}\) is the \(y^\text{th}\) percentile of \(U_{shn}\) presented earlier in this section and \(c\) is the speed of light in vacuum.

Figure 4 shows example one-dimensional cuts at three different time steps taken from a PIC simulation. The simulation parameters are as follows: \(\theta_{in} = 60\) deg, \(\Delta = 6.5\), \(n_{in} = 4\), \(\rho_i = 900\), \(\Delta = 1\) \(\lambda_{De}\) (where \(\Delta\) is the grid cell size), initially 1,000 particles per cell, and \(\lambda_e/\lambda_{De} \sim 8\) (i.e., \(\sim 27\) times smaller than median solar wind values near 1 AU). All of the panels show data in normalized units. The electric field is normalized to the initial upstream averaged convective electric field, \(-\mathbf{E} \times \mathbf{B}\), i.e., the same \(E_v\) referenced for spacecraft observations. Thus, in the upstream the \(E_v\) component has an offset of unity. The normalization for \(n_e\) and \(B\) are just the initial upstream average values of the magnitude of each. All fields are measured in the simulation frame, where the shock moves in the positive \(x\) direction with the speed of approximately \(2V_A\).

One can see that the largest values of \(|E|\) rarely exceed 2 (i.e., only short intervals >2 but peak only at ~6), similar to the simulations discussed previously. Further, the spatial scales at which these fields are maximized is on \(\lambda_e\) scales whereas observations show maximum electric fields at \(\lambda_{De}\) scales. One can also see that the ramp, e.g., \(B\) in panel (D), is about \(L_{sh} \sim 28\) \(\lambda_e\) (or \(\sim 0.9\) \(\lambda_{De}\)) thick, similar to observations that typically show ramps satisfying \(L_{sh} < 35\) \(\lambda_e\) (or \(<0.8\) \(\lambda_{De}\)) (Hobara et al., 2010; Mazelle et al., 2010). The simulation does, however, generate the ubiquitous whistler precursor train upstream of the shock ramp (Wilson et al., 2012; Wilson et al., 2017). Yet it is still not clear what parameter or parameters are controlling the shock ramp thickness and electric field amplitudes at very small spatial scales in simulations.

4 DISCUSSION

We have presented examples illustrating that spacecraft observations of collisionless shocks consistently show \(\delta E \gg E_v\) where \(\delta E\) is due to electrostatic fluctuations satisfying \(k\lambda_{De} \lesssim 1\) with frequencies well above \(f_{pe}\). In contrast, most PIC simulations of collisionless shocks show considerably smaller amplitude of electrostatic fluctuations. This is true even when the simulation uses realistic \(\rho_i/\lambda_{De}\) and plasma betas.

Further, many simulations still generate shock ramps satisfying \(L_{sh}\). \(\lambda_{De}\) > 43, i.e., thicker than most observations. However, much more progress has been made on this front where Yang et al. (2013) concluded that the shock ramp thickness decreased with increasing \(\rho_i/\lambda_{De}\) but increased with increasing ion plasma beta. There is still the question of whether \(\rho_i/\lambda_{De}\) plays a role in the simulated values of \(L_{sh}\), though Yang et al. (2013) was able to produce realistic thicknesses despite only having \(\rho_i/\lambda_{De}\) = 2.

Another potential issue that was not explicitly discussed in detail is that of the separation between \(\lambda_e\) and \(\lambda_{De}\), but these are controlled by \(\rho_i/\lambda_{De}\) and \(\rho_e/\lambda_{De}\). As previously shown, statistical solar wind parameters satisfy \(\lambda_e/\lambda_{De} \sim 215\) (or \(\rho_i/\lambda_{De} \sim 9,757\)) while simulations often have much smaller values of \(\lambda_e/\lambda_{De} \sim 70\)–500 (or \(\rho_i/\lambda_{De} \sim 7\)–40) (Umeda et al., 2011; Umeda et al., 2012a; Umeda et al., 2014; Savoini and Lembègue, 2015). It is also the case that simulations often use shock speeds satisfying \(V_{Te} < V_{Te} < U_{shn} < c\) while shocks in the solar wind tend to satisfy \(V_{Te} < U_{shn} < V_{Te} \ll c\).

The origins of the discrepancy between the observation that \(\delta E \gg E_v\) for electrostatic fluctuations satisfying \(k\lambda_{De} \lesssim 1\) remain unclear. The ratios \(\rho_i/\lambda_{De}\) and \(\rho_e/\lambda_{De}\) are the most likely parameters since they control the separation of spatial and temporal scales between the instabilities of interest and the global shock scales in an obvious manner. A lack of spatial resolution in most simulations may also be a factor. The purpose of this work is to motivate both observational and simulation communities to bridge the gap find closure with this issue. Without an accurate reproduction of the high frequency, large amplitude waves it is not possible to determine at what scales the electric fields dominate the energy dissipation through collisionless shocks.

DATA AVAILABILITY STATEMENT

The datasets presented in this study can be found in online repositories. The names of the repository/repositories and accession number(s) can be found below: https://cdaweb.gsfc.nasa.gov.

AUTHOR CONTRIBUTIONS

LW wrote most of the content and generated all the observational data figures presented herein. L-JC provided critical contributions to simulation techniques and limitations induced by the variation of different normalized parameters.

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Wilson et al. Simulation vs. Observation

Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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