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by

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Modeling of 10 GeV-1 TeV laser-plasma accelerators using Lorentz boosted

simulations

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Modeling of laser-plasma wakefield accelerators in an optimal frame of reference [J.-L. Vay, Phys. Rev. Lett. 98 130405 (2007)] allows direct and efficient full-scale modeling of deeply depleted and beam loaded laser-plasma stages of 10 GeV-1 TeV (parameters not computationally accessible otherwise). This verifies the scaling of plasma accelerators to very high energies and accurately models the laser evolution and the accelerated electron beam transverse dynamics and energy spread. Over 4, 5 and 6 orders of magnitude speedup is achieved for the modeling of 10 GeV, 100 GeV and 1 TeV class stages, respectively. Agreement at the percentage level is demonstrated between simulations using different frames of reference for a 0.1 GeV class stage. Obtaining these speedups and levels of accuracy was permitted by solutions for handling data input (in particular particle and laser beams injection) and output in a relativistically boosted frame of reference, as well as mitigation of a high-frequency instability that otherwise limits effectiveness.

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24 I. INTRODUCTION

Laser plasma accelerators (LPAs) offer order of magnitude increase in accelerating gradient over standard radio-frequency accelerators (which are limited by electrical breakdown), thus holding the promise of much shorter particle accelerators^{1,2}. High quality electron beams of energy up-to 1 GeV have been produced in just a few centimeters³, with 10 GeV stages being planned as modules of a high energy collider^{4,5}.

As a laser propagates through a plasma, it displaces electrons while ions remain essentially 30 static, creating a pocket of positive charges that the displaced electrons rush to fill. The 31 resulting coherent periodic motion of the electrons oscillating around their original position creates a wake (plasma wave) with a periodic structure following the laser. The alternate concentration of positive and negative charges in the wake creates very intense electric fields. An electron (or positron) beam injected with the right phase can be accelerated by those 35 fields to high energy in a much shorter distance than is possible in conventional particle accelerators. The efficiency and quality of the acceleration is governed by several factors 37 which require precise three-dimensional shaping of the plasma column, as well as the laser 38 and particle beams, and understanding of their evolution. 39

Computer simulations have had a profound impact on the design and understanding of 40 past and present LPA experiments⁶⁻⁹, with accurate modeling of wake formation, electron 41 self-trapping and acceleration requiring fully kinetic methods (usually Particle-In-Cell) using large computational resources due to the wide range of space and time scales involved^{7,9}. Fu-43 ture LPA experiments include those that will be carried out using the BELLA (Berkeley lab laser accelerator) facility at LBNL (Lawrence Berkeley National Laboratory), which will use 45 a 40 J, 1 PW laser system to research the production of 10 GeV electron beams in a meterlength plasma¹⁰. Simulations of parameters relevant to such a 10 GeV stage demand as many as 5000 processor hours for a one-dimensional simulation on a NERSC supercomputer¹¹. Various reduced models have been developed to allow multidimensional simulations at manageable computational costs: fluid approximation^{12–14}, quasistatic approximation^{12,15–18}, laser envelope models^{12,14,16,17,19}, and scaled parameters^{20,21}. However, the various approximations that they require result in a narrower range of applicability. As a result, even using several models concurrently does not usually provide a complete description. For example, scaled simulations of 10 GeV LPA stages do not capture correctly some essential transverse physics, e.g. the laser and beam betatron motion, which can lead to inaccurate beam emittance (a measure of the beam quality). An envelope description using a reduce wave operator can capture these effects correctly at full scale for the early propagation through the plasma but can fail as the laser spectrum broadens due to energy depletion as it propagates further in the plasma^{13,19,22}. However, capturing depletion accurately is essential to the design of efficient stages, in order to optimize the transfer of energy from the laser to the wake and particle bunch.

An alternative approach allows for orders of magnitude speedup of simulations, whether 62 at full or reduced scale, via the proper choice of a reference frame moving near the speed 63 of light in the direction of the laser²³. It does so without alteration to the fundamental equations of particle motion or electrodynamics, provided that high-frequency light emitted 65 counter to the direction of propagation of the beam can be neglected. This approach exploits the properties of space and time dilation and contraction associated with the Lorentz 67 transformation. It was shown²³ that the ratio of longest to shortest space and time scales of a system of two or more components crossing at relativistic velocities is not invariant under such a transformation (a laser crossing a plasma is just such a relativistic crossing). Since for simulations based on formulations from first principles, the number of computer operations (e.g., time steps) is proportional to the ratio of the longest to shortest time scale of interest, it follows that such simulations will eventually have different computer runtimes, yet equivalent accuracy, depending solely upon the choice of frame of reference.

The procedure appears straightforward: identify the frame of reference which will min-75 imize the range of space and/or time scales and perform the calculation in this frame. 76 However, several practical complications arise. Most importantly, while the fundamental 77 equations of electrodynamics and particle motion are written in a covariant form, the nu-78 merical algorithms that are derived from them may not retain this property, and calculations 79 in frames moving at different velocities may not be successfully conducted with the use of the exact same algorithms. For example, it was shown²⁴ that calculating the propagation of ultra-relativistic charged particle beams in an accelerator using standard Particle-In-Cell techniques leads to large numerical errors, which were fixed by developing a new particle pusher. The modeling of a LPA stage in a boosted frame involves the fully electromagnetic modeling of a plasma propagating at near the speed of light, for which Numerical Cerenkov^{25,26} is a potential issue. Second, the input and output data are usually known

from, or compared to, experimental data. Thus, calculating in a frame other than the laboratory entails transformations of the data between the calculation frame and the laboratory frame. Third, electromagnetic calculations that include wave propagation will include waves propagating forward and backward in any direction. For a frame of reference moving in the direction of the accelerated beam (or equivalently the wake of the laser), waves emitted by the plasma in the forward direction expand while the ones emitted in the backward direction contract, following the properties of the Lorentz transformation. If one is to resolve both forward and backward propagating waves emitted from the plasma, there is no gain in selecting a frame different from the laboratory frame. However, the physics of interest for a laser wakefield is the laser driving the wake, the wake, and the accelerated beam. Backscatter is weak in the short-pulse regime, and does not interact as strongly with the beam as do the 97 forward propagating waves which stay in phase for a long period. It is thus often assumed 98 that the backward propagating waves can be neglected in the modeling of LPA stages. The 99 accuracy of this assumption has been demonstrated by comparison between explicit codes 100 which include both forward and backward waves and envelope or quasistatic codes which 101 neglect backward waves^{7,21,27}. 102

After the idea and basic scaling for performing simulations of LPAs in a Lorentz boosted frame were published²³, there have been several reports of the application of the technique to various regimes of LPA^{9,11,14,28–34}. Speedups varying between several and a few thousands were reported with various levels of accuracy in agreement between simulations performed in a Lorentz boosted frames and in a laboratory frame. High-frequency instabilities were reported to develop in 2D or 3D calculations, that were limiting the velocity of the boosted frame and thus the attainable speedup^{31,32,35}.

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We presented elsewhere³⁶ numerical techniques that were implemented in the Particle-110 In-Cell code Warp³⁷ for mitigating the short wavelength instability, including a solver with 111 tunable coefficients. A detailed study of the application of these techniques to the simulations 112 of scaled LPA stages also revealed that choosing a frame near the frame of the wakefield 113 as the reference frame allows for more aggressive application of filtering or damping for mitigating short wavelength instabilities, than is possible in laboratory frame simulations³⁶. 115 We showed that this is due to hyperbolic rotation of the laser oscillations in space time, 116 which is another beneficial consequence of the Lorentz transformation when transforming 117 the laser from the laboratory to a boosted frame, in particular for frames near the frame of 118

the wakefield³⁸.

In the present paper, we present accurate modeling of 10 GeV-1 TeV LPA stages with 120 beam loading relevant to laser driven collider designs and stages for upcoming lasers^{5,20,21}, 121 verifying the scaling of efficient, deeply depleted LPAs to very high energies⁴. This is enabled 122 by controlling an instability that develops with high-boost frames by using methods that 123 we developed and presented elsewhere^{36,38}, allowing 2D and 3D simulations of 100 GeV and 124 1 TeV class LPA stages in the wakefield frame, thus achieving the maximum theoretical 125 speedups of over 10⁵ and 10⁶, respectively. Accuracy of the method is demonstrated at 126 the percentage level. This method is used for for the numerical exploration at full scale of the performance of a 10 GeV stage with a 40 J laser, taking accurately into account laser depletion and spectrum broadening, as well as the accelerated electron beam energy spread, 129 and the transverse dynamics of both the laser and the electron beam. 130

The theoretical speedup expected for performing the modeling of a LPA stage in a boosted 131 frame is derived in Section 2. Section 3 summarizes the issues that have limited speedups 132 in previous work and solutions. Accurate modeling of full scale and scaled 10 GeV class 133 stages is demonstrated in Section 4, and the method is used to simulate stages in the 100 134 GeV-1 TeV range in Section 5. The evolution of the laser spectrum with respect to the 135 frame boost is given in Appendix A and the consequences on the choice of the optimal boost 136 are discussed. Enabling techniques that were implemented in Warp for input and output of 137 data in a boosted frame are described in Appendix B. 138

139 II. THEORETICAL SPEEDUP DEPENDENCY WITH THE FRAME 140 BOOST

The obtainable speedup is derived as an extension of the formula that was derived earlier²³, taking in addition into account the group velocity of the laser as it traverses the plasma. In our previous work²³, the laser was assumed to propagate at the velocity of light in vacuum during the entire process, which is a good approximation when the relativistic factor of the frame boost γ is small compared to the relativistic factor of the laser wake γ_w in the plasma. The expression is generalized here to higher values of γ , for which the actual group velocity of the laser in the plasma must be taken into account. We shall show that for a 10 GeV class LPA stage, the maximum attainable speedup is above four orders

of magnitude.

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Assuming that the simulation box is a fixed number of plasma periods long, which implies the use (which is standard) of a moving window following the wake and accelerated beam, the speedup is given by the ratio of the time taken by the laser pulse and the plasma to cross each other, divided by the shortest time scale of interest, that is the laser period. To first order, the wake velocity v_w is set by the 1D group velocity of the laser driver, which in the linear (low intensity) limit, is given by²:

$$v_w/c = \beta_w = \left(1 - \frac{\omega_p^2}{\omega^2}\right)^{1/2} \tag{1}$$

where $\omega_p = \sqrt{(n_e e^2)/(\epsilon_0 m_e)}$ is the plasma frequency, $\omega = 2\pi c/\lambda$ is the laser frequency, n_e is the plasma density, λ is the laser wavelength in vacuum, ϵ_0 is the permittivity of vacuum, c_0 is the speed of light in vacuum, and e and m_e are respectively the charge and mass of the electron.

In the simulations presented herein, the runs are stopped when the last electron beam macro-particle exits the plasma, and a measure of the total time of the simulation is given by

$$T = \frac{L + \eta \lambda_p}{v_w - v_p} \tag{2}$$

where $\lambda_p \approx 2\pi c/\omega_p$ is the wake wavelength, L is the plasma length, v_w and $v_p = \beta_p c$ are 163 respectively the velocity of the wake and of the plasma relative to the frame of reference, 164 and η is an adjustable parameter for taking into account the fraction of the wake which 165 exited the plasma at the end of the simulation. For a beam injected into the n^{th} bucket, η 166 would be set to n-1/2. If positrons were considered, they would be injected half a wake 167 period ahead of the location of the electrons injection position for a given period, and one 168 would have $\eta = n - 1$. The numerical cost R_t scales as the ratio of the total time to the 169 shortest timescale of interest, which is the inverse of the laser frequency, and is thus given 170 by 171

$$R_t = \frac{Tc}{\lambda} = \frac{(L + \eta \lambda_p)}{(\beta_w - \beta_p)\lambda}$$
 (3)

In the laboratory, $v_p = 0$ and the expression simplifies to

$$R_{lab} = \frac{Tc}{\lambda} = \frac{(L + \eta \lambda_p)}{\beta_w \lambda} \tag{4}$$

In a frame moving at βc , the quantities become

$$\lambda_p^* = \lambda_p / \left[\gamma \left(1 - \beta_w \beta \right) \right] \tag{5}$$

$$L^* = L/\gamma \tag{6}$$

$$\lambda^* = \gamma \left(1 + \beta \right) \lambda \tag{7}$$

$$\beta_w^* = (\beta_w - \beta) / (1 - \beta_w \beta) \tag{8}$$

$$v_p^* = -\beta c \tag{9}$$

$$T^* = \frac{L^* + \eta \lambda_p^*}{v_w^* - v_p^*} \tag{10}$$

$$R_t^* = \frac{T^*c}{\lambda^*} = \frac{\left(L^* + \eta \lambda_p^*\right)}{\left(\beta_w^* + \beta\right)\lambda^*} \tag{11}$$

where $\gamma = 1/\sqrt{1-\beta^2}$.

The expected speedup from performing the simulation in a boosted frame is given by the ratio of R_{lab} and R_t^*

$$S = \frac{R_{lab}}{R_t^*} = \frac{(1+\beta)(L+\eta\lambda_p)}{(1-\beta\beta_w)L+\eta\lambda_p}$$
(12)

We note that assuming that $\beta_w \approx 1$ (which is a valid approximation for most practical cases of interest) and that $\gamma << \gamma_w$, this expression is consistent with the expression derived earlier²³ for the LPA case which states that $R_t^* = \alpha R_t/(1+\beta)$ with $\alpha = (1-\beta+l/L)/(1+l/L)$, where l is the laser length which is generally proportional to $\eta \lambda_p$, and $S = R_t/R_T^*$. However, higher values of γ are of interest for maximum speedup, as shown below.

For intense lasers $(a \sim 1)$ typically used for acceleration, the energy gain is limited by dephasing³⁹, which occurs over a scale length $L_d \sim \lambda_p^3/2\lambda^2$. Acceleration is compromised beyond L_d and in practice, the plasma length is proportional to the dephasing length, i.e. $L = \xi L_d$. In most cases, $\gamma_w^2 >> 1$, which allows the approximations $\beta_w \approx 1 - \lambda^2/2\lambda_p^2$, and $L = \xi \lambda_p^3/2\lambda^2 \approx \xi \gamma_w^2 \lambda_p/2 >> \eta \lambda_p$, so that Eq.(12) becomes

$$S = (1+\beta)^2 \gamma^2 \frac{\xi \gamma_w^2}{\xi \gamma_w^2 + (1+\beta) \gamma^2 (\xi \beta/2 + 2\eta)}$$
 (13)

For low values of γ , i.e. when $\gamma << \gamma_w$, Eq.(13) reduces to

$$S_{\gamma < <\gamma_w} = (1+\beta)^2 \gamma^2 \tag{14}$$

Conversely, if $\gamma \to \infty$, Eq.(13) becomes

$$S_{\gamma \to \infty} = \frac{4}{1 + 4\eta/\xi} \gamma_w^2 \tag{15}$$

Finally, in the frame of the wake, i.e. when $\gamma = \gamma_w$, assuming that $\beta_w \approx 1$, Eq.(13) gives

$$S_{\gamma = \gamma_w} \approx \frac{2}{1 + 2\eta/\xi} \gamma_w^2 \tag{16}$$

the speedup that is obtained by using the frame of the wake will be near the maximum obtainable value given by Eq.(15).

Note that without the use of a moving window, the relativistic effects that are at play in the time domain would also be at play in the spatial domain²³, and the γ^2 scaling would transform to γ^4 . In the frame of the wake, there is no need of the moving window, thus simplifying the procedure, while in a frame traveling faster than the wake in the laboratory, a moving window propagating in the backward direction would be needed. However, the

Since η and ξ are of order unity, and the practical regimes of most interest satisfy $\gamma_w^2 >> 1$,

scaling shows that there would be very little gain in doing the latter. Furthermore, analysis presented elsewhere^{36,38} and below show that choosing a frame near the frame of the wake

 $_{201}$ is optimum for mitigation of a high frequency instability. This point is refined by a detailed

 $_{202}$ analysis of the laser spectrum on axis in Appendix A which shows that for heavily depleted

 $_{203}$ $\,$ lasers where the spectrum red-shifts during propagations, the optimal γ might be at a slightly

204 lower value, but this does not greatly affect speedup.

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$_{5}$ A. Estimated speedup for 0.1-100 GeV stages

Formula (13) is used to estimate the speedup for the calculations of 100 MeV to 1 TeV 206 class stages, assuming a laser wavelength $\lambda = 0.8 \mu m$. Parameters for the 100 MeV stage are 207 given in Table 1 below, and parameters for higher energies are derived using scaling laws 208 from $^{20}.$ The initial plasma densities n_e for the 100 MeV, 1 GeV, 10 GeV, 100 GeV and 209 $1~{\rm TeV~stages~are~respectively~10^{19}~cm^{-3},~10^{18}~cm^{-3},~10^{17}~cm^{-3},~10^{16}~cm^{-3}~and~10^{15}~cm^{-3},}$ 210 while the plasma lengths L are 1.5 mm, 4.74 cm, 1.5 m, 47.4 m and 1.5 km if choosing 211 $\xi \approx 1.63$. For these values, the wake wavelengths λ_p are respectively $10.6 \mu \text{m}$, $33.4 \mu \text{m}$, 212 $106.\mu \text{m}$, $334.\mu \text{m}$, 1.06 mm, and relativistic factors γ_w are 13.2, 41.7, 132, 417 and 1320. In 213 the simulations presented in this paper, the beam is injected near the end of the wake period (first "bucket"). The beam has propagated through about half a wake period to reach full 215 acceleration (due to dephasing), and we set $\eta \approx 0.5$. For the parameters considered here, 216 $L \approx \lambda_p/\gamma_w^2$, and (15) gives $S_{\gamma \to \infty} \approx 2\gamma_w^2$.

The speedup versus the relativistic factor of the boosted frame γ is plotted in Fig. 1-a. As 218 expected, for low values of γ , the speedup scales as (14), and asymptotes to a value slightly 219 lower than $2\gamma_w^2$ for large values of γ . Calculations using the frame of the wake $(\gamma = \gamma_w)$ 220 attain nearly the maximum speedup. It is of interest to note that the qualitative behavior 221 is identical to the one obtained in our earlier work²³ (see Fig. 1 and accompanying analysis) in the analysis of the crossing of two rigid identical beams, confirming the generality of the generic analysis presented previously²³. For 10 GeV, 100 GeV and 1 TeV class stages, 224 the maximum estimated speedups are as large as 3×10^4 , 3×10^5 and 3×10^6 respectively. 225 Estimated computational time without boost scales as λ_p^6 (λ_p^3 volume \times λ_p^3 long) $\approx E^3$ (where 226 E is the stage energy) making them harder to model. Fortunately, the boost provides more 227 computational gain for the higher energy stages, making them accessible. 228

III. NUMERICAL ISSUES IN PAST BOOSTED FRAME SIMULATIONS AND OBSERVED SPEEDUPS

Several numerical limits can restrict the boost performance. Here we review limits in past simulations and their impact on performance (a short wavelength instability, laser initialization, statistics), and present methods for circumventing these limits.

A violent numerical instability developing at the front of the plasma column for $\gamma \gtrsim$ 234 100 in 2D and $\gamma \gtrsim 50$ in 3D was reported ^{31,32,35} using the Particle-In-Cell codes Osiris ⁴⁰, 235 Vorpal⁴¹ and Warp³⁷. The presence and growth rate of the instability is observed to be very 236 sensitive to the resolution (slower growth rate at higher resolution), and to the amount of 237 damping of high frequencies and filtering of short wavelengths³⁶. The instability is always 238 propagating at an angle from the longitudinal axis, and is observed in 2D and 3D runs but 239 was never observed in any of the 1D runs. When modeling an LPA setup in a relativistically 240 boosted frame, the background plasma is traveling near the speed of light and it has been 241 conjectured³² that the observed instability might be caused by numerical Cerenkov effect. 242 The instability was studied in detail with Warp and effective mitigation was demonstrated 243 on 10 GeV class LPA stages using newly developed algorithms and results³⁶. 244

Secondly, boosted frame simulations may require larger simulation boxes in the transverse dimension if the entire laser is to be initialized at t = 0, as is common practice for standard laboratory frame simulations^{11,30,32}. The Rayleigh length of the laser is contracted by γ in

the boosted frame, while the laser duration increases by $\gamma(1+\beta)$, implying an increase of the entire laser spot size by $\gamma^2 (1+\beta)^{32}$. If the laser is to be initialized entirely in the simulation 249 box at t = 0, then the simulation box transverse surface increases as $\gamma^4 (1 + \beta)^2$. Although 250 the cost of the simulation does not scale linearly with the simulation box transverse surface, 251 as most of it is used only for laser initialization and does not contain macro-particles, the 252 scaling is so unfavorable that gains of γ^2 provided by the reduction of time steps can be 253 overtaken by the γ^4 additional costs in grid size, thus limiting the usefulness of the method 254 to low values of γ boost. Diagrams of the laser emission procedures used for boosted frame 255 simulations with the Osiris, Vorpal and Warp are given in Fig. 2. Osiris initializes the entire 256 laser at once and is thus subject to the abovementioned limitations. To circumvent those, 257 Vorpal emits the laser from all but one faces of the simulation box¹¹ using total field/scattered 258 field technique⁴², while Warp emits via a moving planar antenna as described in Appendix 259 В. 260

Thirdly, for a given number of plasma macro-particles per cell, the total number of macro-261 particles in the entire plasma column goes down as $1/\gamma^2$ where γ is the relativistic factor 262 of the Lorentz boost³². However, simulations of self-injection regimes require a sufficient 263 number of macro-particles in the plasma column so that adequate statistics ensues in the number of trapped macro-electrons, imposing a ceiling in the value of γ that can be used. 265 For a typical scheme, a $\gamma_{max} \simeq 50$ was derived³² using purely statistical arguments assuming 266 the usage of macro-particles of equal weights. This limit might be relaxed by using varying 267 macro-particle weights such that regions with high probability of trapping (as determined 268 from the accumulated knowledge of previous work) are populated with a higher density of 269 macro-particles of smaller weights. This is already practiced in ordinary runs (i.e. without 270 boosted-frame) for minimizing the computational cost while maximizing the statistics within 271 "dynamically interesting" regions⁴³. For instance it is found^{6,44,45} that in the bubble regime, 272 self-injected particles are initially located within a relatively narrow ring region along the 273 laser axis whose radius is of the order of the laser waist. Previous simulations can be utilized 274 to determine exactly the radius and thickness of the ring region. This issue does not affect 275 the modeling of stages with external injection that will be considered in this paper. 276

Observed speedups from simulations using the Particle-In-Cell codes Osiris, Vorpal and Warp are plotted for 0.1 GeV to 1 TeV stages in Fig. 1-b and contrasted to the theoretical speedups from Eq. (13). All three codes were using the same standard Particle-In-Cell

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method⁴⁶. They all successfully performed 2D and/or 3D calculations with boosts at γ in the range of 20-70, reaching speedups over three orders of magnitude (projected for Osiris assuming no computational cost from laser injection). Without the use of special techniques to mitigate the short wavelength instability, none of the codes could perform successfully 2D or 3D simulations for γ boost values over 100. With the use of the special techniques described elsewhere³⁶ and in Appendix B, Warp simulations were successfully performed using γ boost as high as 1,300 in 2D and 400 in 3D for 1 TeV and 100 GeV class stages respectively.

It is important to note that observed speedups were obtained from simulations of different 288 setups and thus do not offer a direct comparison of the merits of the different codes with regards to boosted frame simulations: Osiris simulations were of trapped self-injection stages, while Vorpal and Warp simulations were of external injection stages with beam loading. 291 Furthermore, while Vorpal and Warp simulations used special procedures to launch the 292 laser that minimize the transverse grid size, Osiris' did not and used transverse grid sizes 293 that were notably larger (as described above). This made Osiris runs in boosted frames 294 substantially more costly, which does not show in the speedups reported by Osiris as this 295 effect was not factored in. However, it is also important to recognize that the most important 296 limiting factor was the high frequency instability (observed in 2D and 3D), which seems to 297 have affected boosted frame simulations of LPA equally, independently of the code used or 298 the simulated LPA setup, legitimizing the comparison in this respect. 299

The numerical techniques that were developed and implemented in Warp³⁶ [as described in Appendix B] are used in the next sections to demonstrate stability and convergence of the boosted frame method up to the 100 GeV-1 TeV range.

$_{303}$ IV. MODELING 10 GEV CLASS LASER PLASMA ACCELERATION $_{304}$ STAGES

This section presents the modeling of deeply depleted and beam loaded 10 GeV LPA stages at full scale in 2-1/2D and 3D using the new numerical techniques that we implemented in Warp in³⁶ and in Appendix B, which has not been done fully self-consistently without the Lorentz boost method.

It has been shown that many parameters of high energy LPA stages can be accurately

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simulated at reduced cost by simulating stages of lower energy gain, with higher density 310 and shorter acceleration distance, by scaling the physical quantities relative to the plasma 311 wavelength, and this has been applied to design of 10 GeV LPA stages^{20,21}. The number 312 of oscillations of a mismatched laser pulse in the plasma channel however depends on stage 313 energy and does not scale, though this effect is minimized for a channel guided stage^{20,21}. 314 The number of betatron oscillations of the trapped electron bunch will also depend on the 315 stage energy, and may affect quantities like the emittance of the beam. For these reasons, 316 and to prove validity of scaled designs of other parameters, it is necessary to perform full 317 scale simulations, which is only possible by using reduced models (e.g., Ref. 19) or simulations 318 in the boosted frame. 319

The basic prescription for scaling a LPA simulation to lower plasma density and higher 320 electron energy gain can be briefly summarized as follows (for additional details see Refs^{20,21}). 321 First, a fully resolved simulation (i.e., sufficient number of grid points per laser wavelength 322 λ) is performed at a relatively low value of $\lambda_p/\lambda = k/k_p$ (i.e., at a relatively high plasma 323 density for a fixed laser wavelength). Next, the simulation results are scaled to a higher 324 value of k/k_p (i.e., lower density) by keeping the normalized laser and beam parameters 325 fixed (constant a_0 , k_pL , $k_p\sigma$, $k_p\sigma_z$, $k_p\sigma_r$, and n_b/n_0 , where a_0 is the laser normalized vector 326 potential, k_p is the plasma wavenumber, n_b is the electron beam density, L and σ are 327 the longitudinal and transverse sizes of the laser, and σ_z and σ_r are the longitudinal and 328 transverse sizes of the beam), since these normalized parameters determine the structure 329 of the accelerating and focusing plasma wakefields. The acceleration length L_d (e.g., the 330 length for the electron beam to reach maximum energy) and the electron energy gain γ_{max} 331 scale as $L_d k_p^3/k^2 = \text{constant}$ and $\gamma_{max} k_p^2/k^2 = \text{constant}$, since the dephasing and depletion 332 lengths scale as $L_d \sim k^2/k_p^3$ and the accelerating field scales as $E_z \sim k_p$. As noted above, 333 some physically relevant quantities do not remain constant when scaled to higher values of 334 k/k_p , such as the trapping threshold for particles in the wake⁴⁷ as well as the normalized 335 Rayleigh length, $k_p Z_R = k k_p \sigma^2/2$, which determines for example the number of oscillations 336 of a mismatched laser pulse in a plasma channel. For this reason, in general, fully resolved 337 simulations at the correct value of k/k_p are still desirable. 338

For benchmarking purposes, scaled simulations²⁰ are performed, first at a density of $n_e = 10^{19} \text{ cm}^{-3}$, using various values of the boosted frame relativistic factor γ to show the accuracy and convergence of the technique. These scaled simulations were shown to

efficiently accelerate both electrons and positrons with low energy spread, and predicted 342 acceleration of hundreds of pC to 10 GeV energies using a 40 J laser. The accuracy of the 343 boosted frame technique is evaluated by modeling scaled stages^{20,21} at 0.1 GeV, which allows 344 for a detailed comparison of simulations using a reference frame ranging from the laboratory 345 frame to the frame of the wake. Excellent agreement is obtained on wakefield histories on axis, beam average energy and transverse RMS size histories, and momentum spread at peak energy, with speedup over a hundred, in agreement with the theoretical estimates from Section 2. The boosted frame technique is then applied in the next section to provide full 349 scale simulation of high efficiency quasilinear LPA stages at higher energy, verifying the 350 scaling laws in the 10 GeV-1 TeV range. 351

352 A. Scaled 10 GeV class stages

The main physical and numerical parameters of the simulations are given in Table I. 353 They were chosen to be close (though not identical) to a case reported elsewhere 20 with 354 $k_pL=2$ where L is the laser pulse length as defined in Table I, the main differences being 355 a sinusoidal versus gaussian laser longitudinal profile and a laser spot size larger by $\sqrt{2}$. 356 These simulations are for a fully resolved 100 MeV stage at a density of 10¹⁹ cm⁻³, which 357 can be scaled to describe a 10 GeV stage at a density of 10^{17} cm⁻³, thereby allowing short 358 run times to permit effective benchmarking between the algorithms^{20,21}. These runs were 359 done using the standard Yee solver with no damping, and with the 4-pass stride-1 filter plus compensation³⁶. No signs of detrimental numerical instabilities were observed at the 361 resolutions reported here with these settings in 2-1/2D or 3D.

For the given parameters, the wake relativistic factor $\gamma_w \approx 13.2$. Thus, Warp simulations 363 were performed using reference frames moving between $\gamma = 1$ (laboratory frame) and 13. 364 For a boosted frame associated with a value of γ approaching γ_w in the laboratory, the 365 wake is expected to travel at low velocity, and the physics to appear somewhat different 366 from that observed in the laboratory frame, in accordance to the properties of the Lorentz 367 transformation³⁸. Figures 3 and 4 show surface renderings of the transverse and longitudinal electric fields respectively, as the beam enters its early stage of acceleration by the plasma 369 wake, from a calculation in the laboratory frame and another in the frame at $\gamma = 13$. The two 370 snapshots offer strikingly different views of the same physical processes: in the laboratory 371

TABLE I. List of parameters for a LPA stage simulation at 100 MeV

plasma density on axis	n_e	10^{19} cm^{-3}
plasma longitudinal profile		flat
plasma length	L_p	1.5 mm
plasma entrance ramp profile		half sine
plasma entrance ramp length		$20~\mu\mathrm{m}$
laser profile		$a_0 \exp\left(-r^2/2\sigma^2\right) \sin\left(\pi z/3L\right)$
normalized vector potential	a_0	1
laser wavelength	λ	$0.8~\mu\mathrm{m}$
laser spot size (RMS)	σ	$8.91~\mu\mathrm{m}$
laser length (HWHM)	L	$3.36~\mu\mathrm{m}$
normalized laser spot size	$k_p\sigma$	5.3
normalized laser length	k_pL	2
beam profile		$n_{b0} \exp\left(-r^2/2\sigma_r^2 - z^2/2\sigma_z^2\right)$
beam transverse size (RMS)	σ_r	165 nm
beam length (RMS)	σ_z	85 nm
normalized beam spot size	$k_p \sigma_r$	0.1
normalized beam length	$k_p \sigma_z$	0.05
beam transverse emittance	ϵ	73.5 nm.mrad
beam total charge (3D)	Q	$6.42~\mathrm{pC}$
beam initial energy	E_0	$1.5\gamma_w m_e c^2$
injection distance after laser max		$0.7\lambda_p$
number of cells in x	N_x	75
number of cells in z	N_z	860 ($\gamma = 13$)-1691 ($\gamma = 1$)
cell size in x	δx	$0.65 \mu m$
cell size in z	δz	$\lambda/64$
time step	δt	at CFL limit
particle deposition order		cubic
# of plasma particles/cell		1 macro-e ⁻ +1 macro-p ⁺

frame, the wake is fully formed before the beam undergoes any significant acceleration and 372 the imprint of the laser is clearly visible ahead of the wake; in the boosted frame calculation, 373 the beam is accelerated as the plasma wake develops, and the laser imprint is not visible on 374 the snapshot. Close examination reveals that the short spatial variations which make the 375 laser imprint at the front of the wake are transformed into time variations in the boosted 376 frame of $\gamma = 13$. This effect is due to hyperbolic rotation in Minkowski space of the laser 377 propagation in plasma, as explained in more detail elsewhere³⁸. The imprint of the beam 378 loading is clearly visible on the plot of the longitudinal electric field (wake) in the laboratory 379 frame (top plot of Figure 4). 380

Histories of the perpendicular and longitudinal electric fields recorded at a number of 381 stations at fixed locations in the laboratory offer direct comparison between the simulations 382 in the laboratory frame ($\gamma = 1$) and boosted frames at $\gamma = 2, 5, 10$ and 13. Figure 5 and 383 6 show respectively the transverse and longitudinal electric fields collected at the positions 384 z=0.3 mm and z=1.05 mm (in the laboratory frame) on axis (x=y=0). The agreement 385 is excellent and confirms that despite the apparent differences from snapshots taken from 386 simulations in different reference frames, the same physics was recovered. The effect of beam 387 loading is visible in Figure 6 at $t \approx 1.15$ ps and $t \approx 3.61$ ps, confirming that the amplitude 388 and phase of beam loading was correctly recovered in all frames. This is further confirmed by the plot of the average scaled beam energy gain and transverse RMS size as a function 390 of position in the laboratory frame, and of relative longitudinal momentum dispersion at 391 peak energy (Fig. 7). These show that the correct laser evolution and electron beam 392 energy, momentum spread and transverse dynamics were modeled in all frames. The small 393 differences observed in the mean beam energy histories and on the longitudinal momentum 394 spread are due to a lack of convergence at the resolution that was chosen, and we have 395 verified that convergence was improving with increasing resolution. The beam was launched 396 with the same phase in the 2-1/2D and the 3D simulations, resulting in lower energy gain 397 in 3D, due to proportionally larger laser depletion effects in 3D than in 2-1/2D. 398

The CPU time recorded as a function of the average beam position in the laboratory frame indicates that the simulation in the frame of $\gamma = 13$ took ≈ 25 s in 2-1/2D and ≈ 150 s in 3D versus $\approx 5,000$ s in 2-1/2D and $\approx 20,000$ s in 3D in the laboratory frame, demonstrating speedups of ≈ 200 in 2-1/2D and ≈ 130 in 3D, between calculations in a boosted frame at $\gamma = 13$ and calculations in the laboratory frame.

All the simulations presented so far in this section were using the Yee solver³⁶, for which the Courant condition is given by $c\delta t < (1/\delta x^2 + 1/\delta z^2)^{-1/2}$ in 2D and $c\delta t < (1/\delta x^2 + 1/\delta y^2 + 1/\delta z^2)^{-1/2}$ in 3D where δt is the time step and δx , δy and δz are the computational grid cell sizes in x, y and z. As γ was varied, the transverse resolution was kept constant, while the longitudinal resolution was kept at a constant fraction of the incident laser wavelength $\delta z = \zeta \lambda$, such that in a boosted frame, $\delta z^* = \zeta \lambda^* = \zeta (1 + \beta) \gamma \lambda$. As a result, the speedup becomes, when using the Yee solver

$$S_{yee2D} = S \frac{\delta z \sqrt{1/\delta x^2 + 1/\delta z^2}}{\delta_z^* \sqrt{1/\delta x^2 + 1/\delta z^{*2}}}$$

$$\tag{17}$$

411 in 2D and

$$S_{yee3D} = S \frac{\delta z \sqrt{1/\delta x^2 + 1/\delta y^2 + 1/\delta z^2}}{\delta_z^* \sqrt{1/\delta x^2 + 1/\delta y^2 + 1/\delta z^{*2}}}$$
(18)

in 3D, where S is given by Eq. (13).

The speedup versus relativistic factor of the reference frame is plotted in Fig. 8, from (13), (17) and (18), and contrasted with measured speedups from 1D, 2-1/2D and 3D Warp simulations, confirming the scaling obtained analytically.

This subsection demonstrated accurate modeling of the evolution of the laser and the electron beam energy, momentum spread and transverse dynamics with agreement at the percentage level between simulations using various reference frames. The scaling of the speedup was also confirmed, validating our understanding of the boosted frame method scaling with γ boost.

B. Full scale 10 GeV class stages

The boosted frame technique was next applied to the modeling of 10 GeV stages at full 422 scale (i.e. at plasma density $n_e = 10^{17} \text{ cm}^{-3}$, with parameters scaled from Table 1). As 423 noted elsewhere¹¹, full scale simulations using the laboratory frame of 10 GeV stages at 424 plasma densities of 10¹⁷ cm⁻³ are not practical on present computers in 2D and 3D. At this 425 density, the wake relativistic factor $\gamma_w \approx 132$, and 2-1/2D and 3D simulations were done 426 in boosted frames up to $\gamma = 130$, realizing the maximum theoretical speedup. This section demonstrates accurate modeling of the particle beam acceleration and transverse dynamics 428 evolution of full scale beam loaded 10 GeV stages in 2D and 3D for boosted frames up to 429 $\gamma = 130.$ 430

Fig. 9 and Fig. 10 show the average beam energy gain and transverse RMS size versus 431 longitudinal position from respectively 2-1/2D and 3D simulations in boosted frames at 432 $\gamma = 30$ to 130 in 2-1/2D and at $\gamma = 60$ to 130 in 3D (runs at $\gamma = 1$ are impractical and 433 were not performed). All runs gave the same beam energy history within a few percent. 434 The average energy gain peaks around 10 GeV in 2-1/2D and 8 GeV in 3D, in agreement 435 with the scaled simulations (see Fig. 7). The abovementioned short wavelength instability that occurs at high values of γ boost is described elsewhere³⁶ and has been mitigated in the 437 3D simulations using $\gamma \geq 120$ using a novel electromagnetic solver and time step $(c\delta t/\delta z =$ 438 $1/\sqrt{2}$) for which the instability growth rate is greatly reduced, completed by smoothing 439 of short wavelengths³⁶. The small discrepancy between the results of the runs at various 440 γ is due to lack of convergence and difficulty in attaining identical initial conditions (see 441 Appendix B) at the resolution that was chosen (32 grid cells per laser wavelength in vacuum). 442 Preliminary scans with varying resolution (not shown here) show that agreement improves 443 with higher resolution and suggest that boosted frame simulations may converge faster than 444 laboratory frame simulations. 445

The boosted frame technique was applied to the direct simulation of a 10 GeV stage 446 $(n_e=10^{17}~{\rm cm}^{-3})$ in which the accelerated charge was sufficiently high so that the effects of 447 beam loading were readily evident. These parameters are relevant to experiments that will 448 be carried out on new lasers, such as the BELLA facility at LBNL¹⁰, and to LPA stages that 449 can serve as the basis for high energy collider modules^{4,5}. In this simulation, a laser pulse 450 with intensity $a_0 = 1.414$, wavelength $\lambda = 0.8$ microns and RMS duration of L/c = 40 fs 451 (i.e. $k_pL = 1/\sqrt{2}$), where L is the longitudinal RMS size of the gaussian laser pulse profile 452 $a(r,z)=a_0\exp\left(-r^2/2\sigma^2-z^2/2L^2\right)$ was focused to a RMS gaussian transverse spot size of 453 63 microns (i.e. $k_p\sigma=3.75$) at the channel entrance. The plasma channel had an on-axis 454 density $n_0 = 10^{17} \text{ cm}^{-3}$, a length of 0.75 m with a parabolic channel (factor=0.6) and a 455 longitudinal taper^{20,48} of the form $n(x) = n_0(1.32x + 1)$. An electron beam with a gaussian 456 profile and 17 microns size (i.e. $k_p\sigma_r=1$) and 8.5 microns length (i.e. $k_p\sigma_z=0.5$) was 457 externally injected at a distance of $1.53\lambda_p$ behind the location of maximum laser intensity 458 with an initial energy of 100 MeV and an initial emittance of 60 mm-mrad. The calculation 459 was in 2-1/2D, and the beam charge density corresponded to a total charge of ~ 52 pC in 460 3D. The large input emittance was chosen to maximize the beam radius for efficient beam 461 loading and for emittance matching to the wakes focusing fields²⁰. Figure 11 shows the 462

density wake excited by an intense laser pulse and the externally injected electron beam 463 accelerated by the wake. The color coding indicates the energy reached by the electrons. 464 The depression in the density wake is due to self-consistent beam loading of the injected 465 electron bunch. The histories of electron beam mean energy, emittance and RMS size are 466 given in Figure 12, while the longitudinal momentum distribution is given in Figure 13. At the exit of the structure, electrons with energy of up to 11 GeV were observed. The time projected energy spread and normalized emittance when exiting the plasma channel were 469 15% and 61 mm-mrad, respectively. The slice energy spread and emittance of a slice at 470 $9.5~{
m GeV}$ were 1% and $54~{
m mm}$ -mrad. Whereas these values are larger than acceptable for 471 collider and light source applications, it has been shown that lower emittance bunches can be 472 accelerated by using high order laser modes to control the transverse focusing forces⁴⁹ and 473 lower energy spread by controlling beam loading^{20,50}. Future work will aim at optimizing 474 the phase space properties of the bunch including optimization of taper⁴⁸ and use of higher 475 order laser modes to minimize emittance. 476

The present work demonstrates the ability to simulate at full scale a 10 GeV stage that
exhibits significant laser depletion and beam loading. It confirms that the electron beam
acceleration and energy gain is very well predicted by scaled simulations, and shows that
emittance conservation is obtained through good matching, which is only accurately accounted for at full scale.

482 V. FULL SCALE 100 GEV-1 TEV STAGES

The numerical techniques that we developed³⁶ and successfully applied to the modeling 483 of 10 GeV class stages in the preceding section are applied in this section to the modeling of 484 stages in the 0.1 GeV-1 TeV range in 2-1/2D and in the 0.1-100 GeV range in 3D, showing 485 scaling of LPAs to high energies. The plasma density n_e scales inversely to the energy gain, 486 from $10^{19}~{\rm cm^{-3}}$ down to $10^{15}~{\rm cm^{-3}}$ in the 0.1 GeV-1 TeV range. These simulations used 487 the parameters given in Table I scaled appropriately to higher energies²⁰, and used the high 488 speed of the boosted simulations to allow fast turnaround improvement of the stage design 480 presented in 20,21 . 490

The average beam energy gain history is plotted in Fig. 14, scaling the 0.1-100 GeV runs to the 1 TeV run in 2-1/2D, and the 0.1-10 GeV runs to the 100 GeV run in 3D. The

differences at 10^{19} cm⁻³ of the scaled beam energy gain history can be attributed to the effects from having only a few laser oscillations per pulse.

Using (13), the speedup of the full scale 100 GeV class run, which used a boosted frame of $\gamma = 400$ as frame of reference, is shown to be over 100,000, as compared to a run using the laboratory frame. Assuming the use of a few thousands of CPUs, a simulation that would require several decades to complete using standard PIC techniques in the laboratory frame, was completed in four hours using 2016 CPUs of the Cray system at NERSC. Also using (13), the speedup of the 2-1/2D 1 TeV stage is shown to be over a million.

This section demonstrated the scaling of highly depleted beam loaded stages up to 1 TeV in 2D and 100 GeV in 3D, providing greater credibility for evaluation of various LPA based collider options⁴.

4 VI. CONCLUSIONS

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Calculations using an optimal boosted frame of 10 GeV, 100 GeV and 1 TeV class stages including beam loading were presented, with speedups over 4, 5 and 6 orders of magnitude respectively over what would be required by "standard" laboratory frame calculations, which are impractical for such stages due to computational requirements. Our previous theoretical speedup estimate²³ was extended to high boost values, while complications associated with the handling of input and output data between a boosted frame and the laboratory frame were discussed. Practical solutions were implemented, including a technique for injecting the laser that is simpler and more efficient than methods proposed previously.

The boosted frame Particle-In-Cell technique has been shown to accurately model the 513 laser evolution and resolve the wavelength shifting and broadening (as described in Appendix 514 A) that occurs as the laser depletes, offering advantages over other models (for example 515 envelope, quasistatic) while providing the speed required for direct simulation of 10 GeV and 516 beyond laser plasma accelerators to accurately model laser and beam transverse oscillations. 517 It has been shown to also model accurately the electron beam acceleration, longitudinal 518 and transverse dynamics. The results are within a few percent of those from 'standard' laboratory frame simulations, which is within acceptable range for the design of proof-of-520 principle experiments. The boosted frame technique is being applied to the direct simulation 521 of 10 GeV beam loaded stages, which is relevant to experiments on new lasers (e.g., the 522

BELLA facility at LBNL), as well as next generation controlled laser plasma accelerator stages and collider modules.

525 VII. ACKNOWLEDGMENTS

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Appendix A: Laser spectrum on axis and optimal frame

In this section, we discuss in more detail how the choice of the optimal frame for smoothing is determined by the laser spectrum. It was shown previously³⁸ that choosing γ boost near γ of the wakefield is a possible option. We extend the discussion to consider depletion of the laser and show that in this case a lower value of γ boost might be desirable.

The spectrum history of the laser field on axis is given in Fig. 15 for selected values of γ between 1 and 135. The history is given up to the time of the electron beam peak energy. In the laboratory frame at $\gamma = 1$, the initial (t=0) spectral content is very localized in a narrow band around the laboratory frame vacuum laser wavelength λ_0 , spreading and redshifting as the laser propagates and depletes its energy into the wake². Although it is not visible in the spectrum, the laser waves propagate in the positive direction in the laboratory frame.

At higher values of γ frame, the initial spectral content of the laser shifts to longer wave-542 lengths relative to the boosted frame vacuum laser wavelength λ'_0 . As the frame approaches 543 the wake frame $\gamma_w \approx 132$, the initial spectrum is displaced toward very long wavelengths 544 (standing waves), because the frame is moving near the laser group velocity. At later times, 545 the high γ frame spectra show content repopulating progressively shorter wavelengths. This corresponds to the redshifting observed in the lab frame; with the calculation frame matching the initial laser group velocity, the redshifted light which propagates slower now slips 548 backward in the moving frame. As γ frame rises, eventually all waves propagate in the 549 negative direction for $\gamma \geq \gamma_w$. 550

Mitigation of the short wavelength instability necessitates higher amounts of smoothing 551 at higher γ , and smoothing is most effective (and has minimal effect on simulation physics) 552 when spectral content is confined to long wavelengths³⁶. This occurs for $\gamma \approx \gamma_w$ initially, and 553 Fig. 15 indicates how for strongly depleted stages the optimum γ may be adjusted slightly 554 below γ_w , in order to maximize the wavelengths of the average spectral content over the 555 propagation length rather than only at the start. The plasma column also usually exhibits 556 a parabolic transverse profile so as to provide transverse focusing of the laser, which also 557 slightly reduces group velocity². These corrections to the optimal gamma are relatively small 558 and thanks to the weak dependency of the speedup with γ near γ_w (cf Fig. 1), simulations 559 with γ approaching γ_w offer speedups that are very near the maximum attainable, thus 560 offering in practice the maximum benefit of the boosted frame technique while maintaining 561 the highest level of accuracy. Other effects such as tapering of the plasma density may 562 further decrease the optimal γ for smoothing. A large value of γ boost can still be used for 563 high energy stages, thus achieving orders of magnitude speedups in practice. 564

At higher resolution, the instability level is reduced³⁶, and so is the amount of smoothing 565 that is necessary to control it. Furthermore, the instability spectrum is confined to a very 566 narrow band located near the Nyquist cutoff of the simulation grid³⁶, and thus separates 567 further from the spectrum with physical content of interest as resolution increases. Hence 568 high resolution simulations may use γ boost near γ wake and achieve maximum speedup 569 even for runs using a tapered plasma. Simulations have been conducted at up to three times 570 the base resolution, where use of $\gamma = \gamma_w$ is possible even including the above effects. The boosted frame speedup allows such high resolutions which may be important for evaluation of future low emittance stage concepts. 573

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Appendix B: Input and output to and from boosted frame simulations in Warp

This section describes the procedures that have been implemented in the Particle-In-Cell 575 framework Warp³⁷ to handle the input and output of data between the frame of calculation 576 and the laboratory frame. Simultaneity of events between two frames is valid only for a 577 plane that is perpendicular to the relative motion of the frame. As a result, the input/output 578 processes involve the input of data (particles or fields) through a plane, as well as output 579 through a series of planes, all of which are perpendicular to the direction of the relative 580

velocity between the frame of calculation and the other frame of choice.

582 1. Input

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583 a. Particles

Particles are launched through a plane using a technique which applies to many calcu-584 lations in a boosted frame, including LPA, and is illustrated using the case of a positively 585 charged particle beam propagating through a background of cold electrons in an assumed 586 continuous transverse focusing system, leading to a growing transverse instability²³. In the 587 laboratory frame, the electron background is initially at rest and a moving window is used 588 to follow the beam progression. Traditionally, the beam macroparticles are initialized all 589 at once in the window, while background electron macroparticles are created continuously 590 in front of the beam on a plane that is perpendicular to the beam velocity. In a frame moving at some fraction of the beam velocity in the laboratory frame, the beam initial conditions at a given time in the calculation frame are generally unknown and one must 593 initialize the beam differently. However, it can be taken advantage of that the beam initial 594 conditions are often known for a given plane in the laboratory, either directly, or via sim-595 ple calculation or projection from the conditions at a given time. Given the position and 596 velocity $\{x, y, z, v_x, v_y, v_z\}$ for each beam macroparticle at time t = 0 for a beam moving at 597 the average velocity $v_b = \beta_b c$ (where c is the speed of light) in the laboratory, and using 598 the standard synchronization (z = z' = 0) at t = t' = 0 between the laboratory and the 599 calculation frames, the procedure for transforming the beam quantities for injection in a 600 boosted frame moving at velocity βc in the laboratory is as follows (the superscript ' relates 601 to quantities known in the boosted frame while the superscript * relates to quantities that 602 are know at a given longitudinal position z^* but different times of arrival): 603

1. project positions at $z^* = 0$ assuming ballistic propagation

$$t^* = \left(z - \bar{z}\right)/v_z \tag{B1}$$

$$x^* = x - v_x t^* \tag{B2}$$

$$y^* = y - v_u t^* \tag{B3}$$

$$z^* = 0 \tag{B4}$$

the velocity components being left unchanged,

2. apply Lorentz transformation from laboratory frame to boosted frame

$$t'^* = -\gamma t^* \tag{B5}$$

$$x^{\prime *} = x^* \tag{B6}$$

$$y'^* = y^* \tag{B7}$$

$$z^{\prime *} = \gamma \beta c t^* \tag{B8}$$

$$v_x^{\prime *} = \frac{v_x^*}{\gamma \left(1 - \beta \beta_b\right)} \tag{B9}$$

$$v_y^{\prime *} = \frac{v_y^*}{\gamma \left(1 - \beta \beta_b\right)} \tag{B10}$$

$$v_z^{\prime *} = \frac{v_z^* - \beta c}{1 - \beta \beta_b} \tag{B11}$$

where $\gamma = 1/\sqrt{1-\beta^2}$. With the knowledge of the time at which each beam macroparticle crosses the plane into consideration, one can inject each beam macroparticle in the simulation at the appropriate location and time.

3. synchronize macroparticles in boosted frame, obtaining their positions at a fixed t'(=0) which is before any particle is injected

$$z' = z'^* - \bar{v}_z'^* t'^* \tag{B12}$$

This additional step is needed for setting the electrostatic or electromagnetic fields at the plane of injection. In a Particle-In-Cell code, the three-dimensional fields are calculated by solving the Maxwell equations (or static approximation like Poisson, Darwin or other²⁴) on a grid on which the source term is obtained from the macroparticles distribution. This requires generation of a three-dimensional representation of the beam distribution of macroparticles at a given time before they cross the injection plane at z'^* . This is accomplished by expanding the beam distribution longitudinally such that all macroparticles (so far known at different times of arrival at the injection plane) are synchronized to the same time in the boosted frame. To keep the beam shape constant, the particles are "frozen" until they cross that plane: the three velocity components and the two position components perpendicular to the boosted frame velocity are kept constant, while the remaining position component is advanced at the

average beam velocity. As particles cross the plane of injection, they become regular "active" particles with full 6-D dynamics.

Figure 16 (top) shows a snapshot of a beam that has passed partly through the injection plane. As the frozen beam macroparticles pass through the injection plane (which moves opposite to the beam in the boosted frame), they are converted to "active" macroparticles.

The charge or current density is accumulated from the active and the frozen particles, thus ensuring that the fields at the plane of injection are consistent.

631 **b.** Laser

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Similarly to the particle beam, the laser is injected through a plane perpendicular to the axis of propagation of the laser (by default z). The electric field E_{\perp} that is to be emitted is given by the formula

$$E_{\perp}(x, y, t) = E_0 f(x, y, t) \sin \left[\omega t + \phi(x, y, \omega)\right]$$
(B13)

where E_0 is the amplitude of the laser electric field, f(x, y, t) is the laser envelope, ω is the laser frequency, $\phi(x, y, \omega)$ is a phase function to account for focusing, defocusing or injection at an angle, and t is time. By default, the laser envelope is a three dimensional gaussian of the form

$$f(x, y, t) = e^{-(x^2/2\sigma_x^2 + y^2/2\sigma_y^2 + c^2t^2/2\sigma_z^2)}$$
(B14)

where σ_x , σ_y and σ_z are the dimensions of the laser pulse; or it can be defined arbitrarily by the user at runtime. If $\phi(x, y, \omega) = 1$, the laser is injected at a waist and parallel to the axis z.

If, for convenience, the injection plane is moving at constant velocity $\beta_s c$, the formula is modified to take the Doppler effect on frequency and amplitude into account and becomes

$$E_{\perp}(x, y, t) = (1 - \beta_s) E_0 f(x, y, t)$$

$$\times \sin \left[(1 - \beta_s) \omega t + \phi(x, y, \omega) \right]. \tag{B15}$$

The injection of a laser of frequency ω is considered for a simulation using a boosted frame moving at βc with respect to the laboratory. Assuming that the laser is injected at a

plane that is fixed in the laboratory, and thus moving at $\beta_s = -\beta$ in the boosted frame, the injection in the boosted frame is given by

$$E_{\perp}(x', y', t') = (1 - \beta_s) E'_0 f(x', y', t')$$

$$\times \sin \left[(1 - \beta_s) \omega' t' + \phi(x', y', \omega') \right]$$

$$= (E_0/\gamma) f(x', y', t')$$

$$\times \sin \left[\omega t' / \gamma + \phi(x', y', \omega') \right]$$
(B16)
(B17)

since $E_0'/E_0 = \omega'/\omega = 1/(1+\beta)\gamma$.

The electric field is then converted into currents that get injected via a 2D array of macro-particles, with one positive and one dual negative macro-particle for each array cell in the plane of injection, whose weights and motion are governed by $E_{\perp}(x',y',t')$. Injecting using this dual array of macroparticles offers the advantages of automatically including the 652 longitudinal component which arise from emitting into a boosted frame, and to automatically 653 verify the discrete Gauss' law thanks to using the Esirkepov current deposition scheme⁵¹. 654 As discussed in section III, the technique implemented in Warp presents several advan-655 tages over other procedures that have been proposed elsewhere 11,32. The method presented 656 here avoids the caveat of the broadening of the transverse size of the laser while retaining 657 simplicity and versatility by injecting through one plane rather than several faces of the box. 658

559 2. Output

Some quantities, e.g. charge or dimensions perpendicular to the boost velocity, are 660 Lorentz invariant. Those quantities are thus readily available from standard diagnostics 661 in the boosted frame calculations. Quantities which do not fall in this category are recorded 662 at a number of regularly spaced "stations", immobile in the laboratory frame, at a succession 663 of time intervals to record data history, or averaged over time. A visual example is given 664 on Fig. 16 (bottom). Since the space-time locations of the diagnostic grids in the labo-665 ratory frame generally do not coincide with the space-time positions of the macroparticles 666 and grid nodes used for the calculation in a boosted frame, some interpolation is performed 667 at runtime during the data collection process. As a complement or an alternative, selected 668 particle or field quantities are dumped at regular interval for post-processing. The choice of 669 the methods depends on the requirements of the diagnostics and particular implementations. 670

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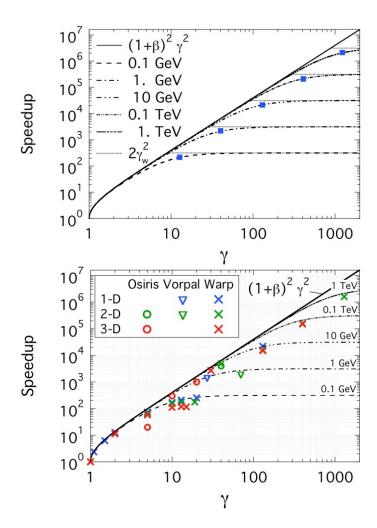


FIG. 1. (top) Theoretical speedup from Eq.(13) versus relativistic factor of the boosted frame for 0.1 GeV - 1 TeV LPA class stages (squares indicate speedup obtained using the frame of the wake $\gamma = \gamma_w$); (bottom) observed speedups from simulations using the code Osiris (circles), Vorpal (triangles) and Warp (crosses) and theoretical speedups (lines) for 0.1 GeV to 1 TeV stages. Vorpal reported speedups courtesy of D. L. Bruhwiler, Tech-X Corp., USA. Osiris reported speedups courtesy of S. F. Martins, IST, Portugal, and W. B. Mori, UCLA, USA.

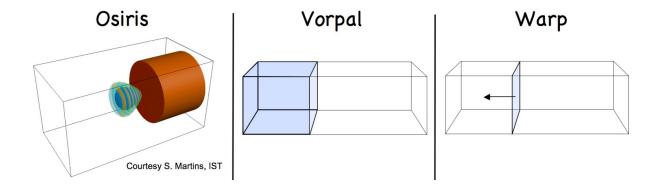


FIG. 2. (color online) Diagrams of laser emission procedures in the Particle-In-Cell codes Osiris (left), Vorpal (middle) and Warp (right) for Lorentz boosted frame simulations. Osiris initializes the entire laser at once. Vorpal emits the laser from all but one faces (blue) of the simulation box. Warp emits through a moving plane (blue). For all three diagrams, the laser propagates from left to right. Reprinted with permission from J.-L. Vay et al., *Proc.* 14th Workshop Advanced Accelerator Concepts. Copyright 2010 American Institute of Physics.

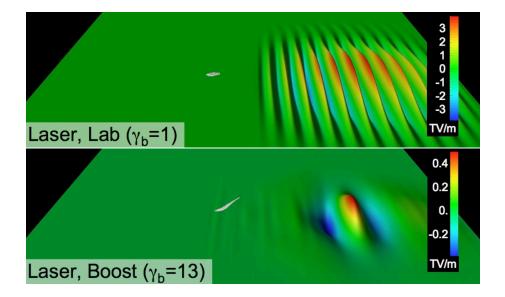


FIG. 3. (color online) Colored surface rendering of the transverse electric field from a 2-1/2D Warp simulation of a laser wakefield acceleration stage in the laboratory frame (top) and a boosted frame at $\gamma = 13$ (bottom), with the beam (white) in its early phase of acceleration. The laser and the beam are propagating from left to right.

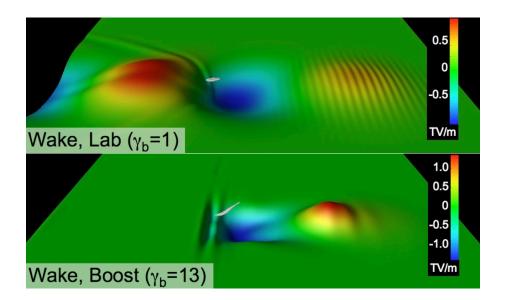


FIG. 4. (color online) Colored surface rendering of the longitudinal electric field from a 2-1/2D Warp simulation of a laser wakefield acceleration stage in the laboratory frame (top) and a boosted frame at $\gamma = 13$ (bottom), with the beam (white) in its early phase of acceleration. The laser and the beam are propagating from left to right.

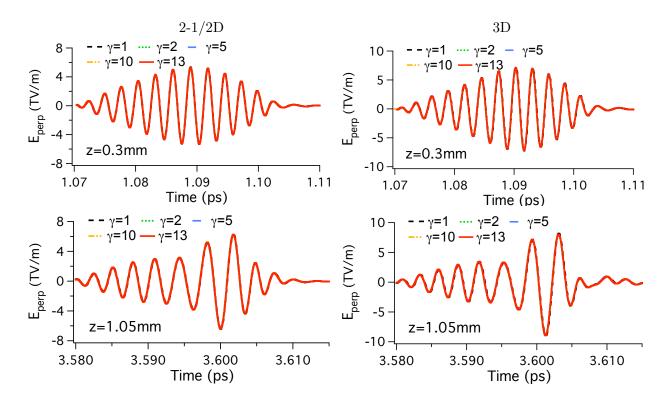


FIG. 5. (color online) History of transverse electric field at the position x=y=0, z=0.3 mm and z=1.05 mm (in the laboratory frame) from simulations in the laboratory frame ($\gamma=1$) and boosted frames at $\gamma=2, 5, 10$ and 13.

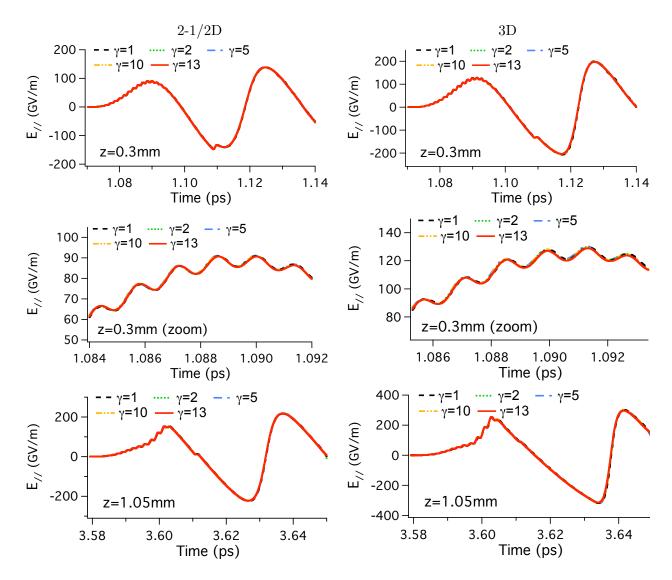


FIG. 6. (color online) History of longitudinal electric field at the position x=y=0, z=0.3 mm and z=1.05 mm (in the laboratory frame) from simulations in the laboratory frame ($\gamma=1$) and boosted frames at $\gamma=2, 5, 10$ and 13.

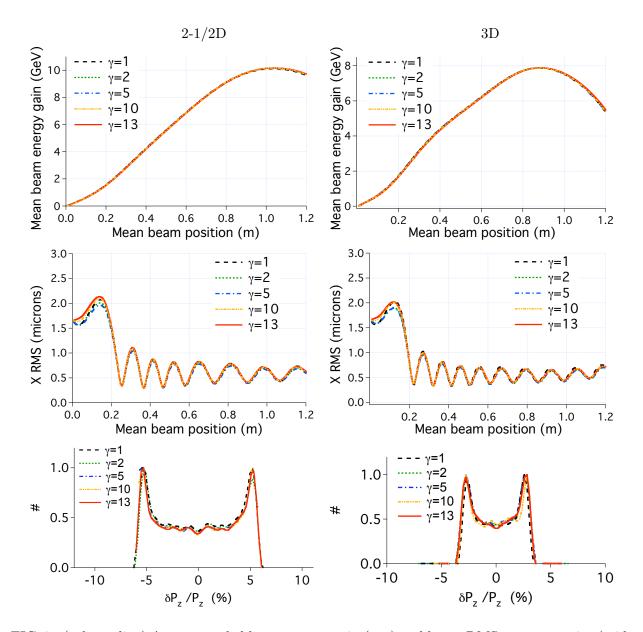


FIG. 7. (color online) Average scaled beam energy gain (top) and beam RMS transverse size (middle) versus longitudinal position in the laboratory frame from simulations; (bottom) distribution of relative longitudinal momentum dispersion at peak energy, in the laboratory frame ($\gamma = 1$) and boosted frames at $\gamma = 2$, 5, 10 and 13.

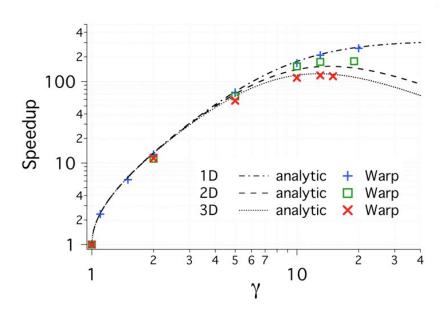


FIG. 8. (color online) Speedup versus relativistic factor of the boosted frame in 1D, 2D and 3D from theoretical estimates (Eq. (13), (17), (18)), and Warp simulations.

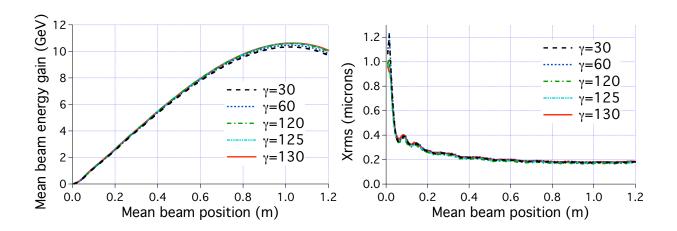


FIG. 9. (color online) Average beam energy gain and transverse size versus longitudinal position (in the laboratory frame) from 2D-1/2 simulations of a full scale 10 GeV LPA in a boosted frame at $\gamma = 30$, 60 and 130, using the Yee solver.

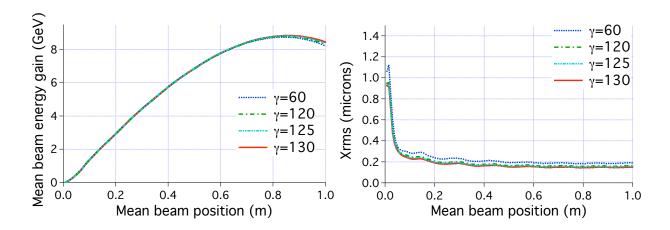


FIG. 10. (color online) Average beam energy gain and transverse size versus longitudinal position (in the laboratory frame) from 3D simulations of a full scale 10 GeV LPA in a boosted frame at $\gamma = 30$, 60, 120, 125 and 130, using the Yee solver ($\gamma = 30$ and 60) and the CK2 solver ($\gamma = 120-130$), with digital filter S(1) and with the time step set by $c\delta t/\delta z = 1/\sqrt{2}$ for stability³⁶.

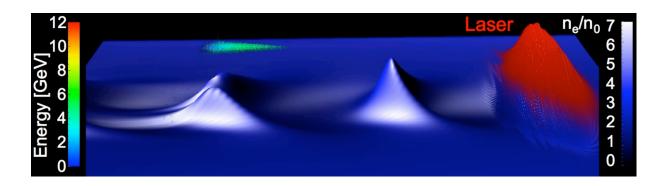


FIG. 11. (color online) Snapshot from a 2-1/2D 10 GeV LPA stage boosted frame simulation as the beam is halfway through acceleration. The image shows an externally injected electron bunch (middle) riding a density wake excited by an intense laser pulse (right), propagating in a 0.75 m long plasma channel.

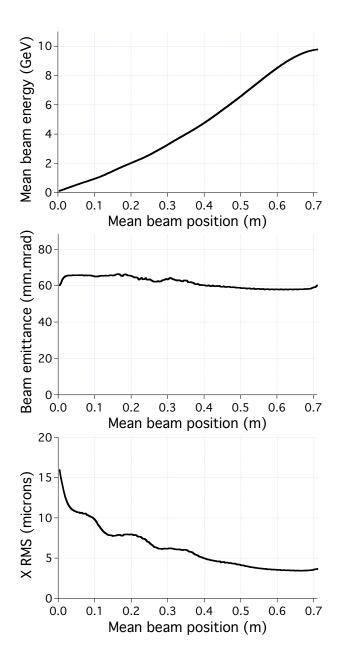


FIG. 12. (top) Average electron beam energy gain, (middle) beam emittance, and (bottom) beam RMS size, versus longitudinal position (in the laboratory frame) from a 2D 10 GeV LPA stage boosted frame simulation.

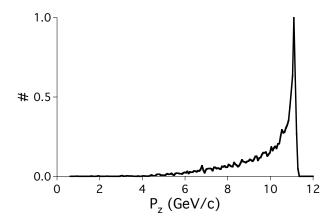


FIG. 13. Longitudinal momentum distribution of the electron beam at maximum energy (z=0.7 m) from a 2D 10 GeV LPA stage boosted frame simulation.

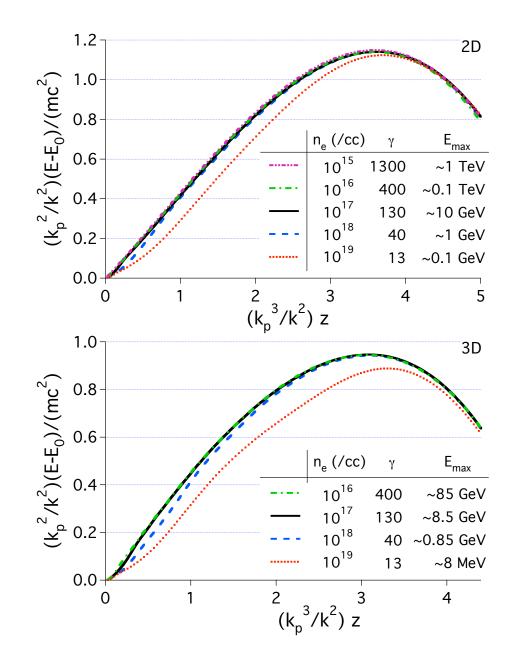


FIG. 14. (color online) Average beam energy gain versus longitudinal position (in the laboratory frame) for simulations at $n_e = 10^{19} \text{ cm}^{-3}$ down to 10^{15} cm^{-3} , using frames of reference between $\gamma = 13$ and $\gamma = 1300$, in 2-1/2D (top) and 3D (bottom).

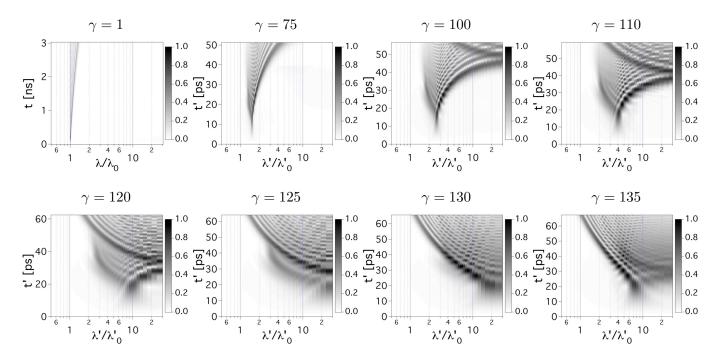


FIG. 15. Spectrum history of the laser field on axis of a 10 GeV stage for selected values of γ between 1 and 135, given up to the time of the electron beam peak energy. The length scale (horizontal axis) is normalized relative to the vacuum laser wavelength as given in each respective frame.

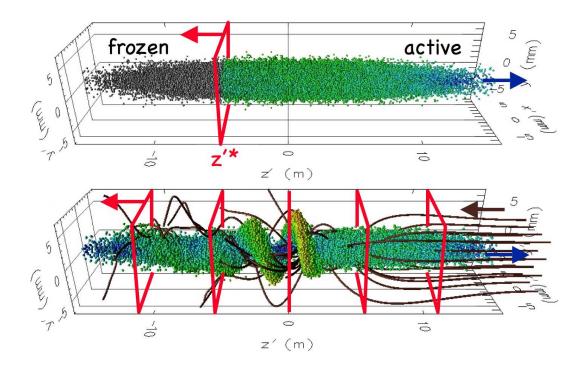


FIG. 16. (color online) (top) Snapshot of a particle beam showing "frozen" (grey spheres) and "active" (colored spheres) macroparticles traversing the injection plane (red rectangle). (bottom) Snapshot of the beam macroparticles (colored spheres) passing through the background of electrons (dark brown streamlines) and the diagnostic stations (red rectangles). The electrons, the injection plane and the diagnostic stations are fixed in the laboratory plane, and are thus counterpropagating to the beam in a boosted frame.