Final Scientific/Technical Report

Continuation of Full-Scale Three-Dimensional Numerical Experiments on High-Intensity Particle and Laser Beam Matter Interactions

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Summary:

Under this grant, we have carried out theory and simulations on fundamental processes in high-intensity laser and particle beam interactions. The simulations have both tested new theories as well as modeled the full-scale in three dimensions of ongoing experiments.

A summary of the highlights during this six year grant that were fully or partially supported under it include:

1. Development of QuickPIC a new quasi-static parallel PIC code including field ionization and ponderomotive guiding center modules including adding the capability of running efficiently on thousands of processors through a novel pipeline algorithm[Huang:2006][Feng:2008].
2. Continued development of OSIRIS including its postprocessing diagnostic and visualization package[Hemker:1999][Fonseca:2002][Martins:2005][Fonseca:2008].
3. Prediction that mono-energetic >100 MeV self-injected electrons could be produced by LWFA using 15TW class 50fs lasers [Tsung:2004, Tsung:2006].
4. Full-scale modeling of PWFA experiments at SLAC [Muggli:2004], [Hogan:2005], [O'Connell:2006], [Johnson:2006], [Oz:2007], [Blumenfeld:2007], [Muggli:2008] and LWFA experiments at Rutherford Appleton Laboratory (RAL)[Mangles:2006], [Willingale:2006], [Thomas:2007], [Kneip:2008], University of Michigan, LBNL, LBNL, UCLA [Ralph:2008] and LLNL[Froula:2008].
5. Full-scale simulations which extrapolate the PWFA experiments towards doubling the energy of 500GeV beams to 1 TeV [Huang:2005].
6. Full-scale simulations to optimize a 25GeV electron PWFA stage for a linear collider[Huang:2008].

7. Development of a theoretical description of nonlinear, and multi-dimensional wakes [Lu:2006a, Lu:2006b].
8. Development of a new theory for electron hosing of short-pulse electron beams [Huang:2007].
9. Development of scaling laws for LWFA in the blowout regime [Lu:2007].
10. First implementation of a Lorentz boosted frame simulations of LWFA [Martins:2008].
11. Full-scale simulations by OSIRIS which extrapolate the LWFA experiments towards generating 12 GeV self-injected electron beams in the self-guided blowout regime [Martins:2008].
12. Full-scale simulations by QuickPIC which extrapolate the LWFA experiments towards generating 100 GeV externally-injected electron beams [Tzoufras:2008a].
13. Development of a nonlinear wakefield beam loading theory in the blowout regime [Tzoufras:2008b].
14. Discovery of electron beam head erosion in self-ionized plasma [Zhou:2008].
15. Development of a detailed understanding self-injection and optimizing the transformer ratio in the blowout regime. [Lu:2008:a][Lu:2008:b][Lu:2008:c].
16. The graduation of two PhD students who were partially supported by this grant.

We have published extensively. We highlight some of the work that has been published during just the last three years including 20 in PRL, 2 in Nature, and 1 in Nature Physics in which the research was partially or fully supported by this award.

A. Continued development of OSIRIS: This grant partially supported the continued to develop OSIRIS. The development was substantial. The development included static as well as dynamic load balancing (in 1D), perfectly matched layers for open EM boundary conditions, a collision package, higher order splines and current smoothing and compensation for improved energy conservation, and improved diagnostics. In addition, we have developed the capability to model laser wakefield stages in a Lorentz boosted frame.

B. The development of QuickPIC: This grant partially supported the development of a new PIC code that is optimized for studying short pulse laser and beam plasma interactions. This code is described in an article that appeared in J. Comp. Phys [Huang:2006]. In figure 1 we show comparisons between QuickPIC and OSIRIS for electron beam drivers, positron beam drivers, electron beam drivers with field ionization

and a laser driver. The agreement is remarkable and the QuickPIC runs require only 100-1000 times less CPU time. The code was continually improved including the addition of a radiation reaction force for the relativistic beams, the addition of a pipelining algorithm [Feng:2008] for greatly improved parallel scaling, and the addition of options in the iterative solver.

Figure 1 :Comparisons between QuickPIC and OSIRIS for electron beam driver (upper left), positron beam driver (upper right), electron beam driver in field-ionized plasma (lower left), and a laser driver with $a_0=2$ (lower right).

Figure 1:

C. Full-scale modeling of PWFA experiments:

During the period of this grant, we have been involved in collaboration between SLAC/UCLA/USC in which high-energy density physics issues related to intense particle beam-matter interactions have been systematically studied in experiments using the electron and positron beams at SLAC. In these experiments the e- or e+ beam has an energy of ~ 28.5 GeV and consists of $\sim 2 \times 10^{10}$ particles. The pulse length is ~ 10 -50 μm and the spot size is 10 μm . This highly productive collaboration has led to numerous publications including 10 Physical Review Letters and two Nature articles on topics ranging from electron and positron acceleration, electron and positron focusing, x-ray emission, and particle beam refraction. A key piece to this collaboration has been full-scale PIC modeling. The development of QuickPIC has made a dramatic difference. One example is shown in figure 2. On the left is an experimental image of the incoming beam dispersed in energy (vertical axis) and one transverse direction (horizontal axis). The beam entered the plasma with a energy spread (the front of the beam of the beam has higher energy). The left image is taken when the plasma is off. On the right is the same images taken from a simulation which used the best guess for the beam and plasma profiles. The simulation showed 4.5 GeV energy gain vs. the experiment which showed 4 GeV energy gain.

Figure 2: Results from the E-164x collaboration. Plots of energy vs. one transverse coordinate of the beam are shown. On the left are experimental results while on the right are the corresponding simulation results.

These set of experiments, culminated with the demonstration that the energy of electrons in the tail of the 42 GeV SLAC beam could be doubled while surfing on the wake excited by electrons in the head of the beam in only .8 meters[Blumenfeld:2007]! For longer plasma lengths the energy gain was actually less. QuickPIC simulations supported under this grant provided the explanation for the saturation in energy gain. It was due to a new effect we called ionization induced head erosion. The experimental results together with full scale simulation results were published in Nature and were featured in a news and views article in a subsequent issue. A comparison between the simulation and experimental data is shown in figure 3.

Figure 3: On the left, energy spectrum from the energy doubling experiment published in Nature and its comparison with QuickPIC simulation. On the right, the comparison of energy gain for different plasma length between experiment and simulation.

D. Full scale modeling of LWFA experiments:

During the grant period, we have extensively used OSIRIS to model ongoing and future LWFA experiments throughout the world. We set out to understand what would happen when lasers in the 5-25 TW and 30-50fs range were sent through uniform plasmas or plasma channels by using high-fidelity full-scale 3D PIC simulations. We were motivated by the realization that several groups in the world would have just such lasers and the

appropriate plasma sources and diagnostics. We simulated a 16TW, 50fs laser propagating through a $3 \times 10^{18} \text{cm}^{-3}$ plasma channel. We were surprised to find that although the initial laser intensity and profile were not sufficient to self-inject or trap plasma electrons that eventually the laser intensity increased to produce mono-energetic, 280 MeV beams with .1nC of charge. Detailed analysis of the simulations indicated that this occurred through a highly nonlinear process involving a combination of photon acceleration (frequency down-shifting) and group velocity dispersion. This led to the laser intensity and pulse shape evolving such that the wake was eventually driven to sufficient amplitudes to self-inject electrons. The electrons then formed a mono-energetic bunch due to phase space rotation as the first part of the bunch dephased. We also saw a second bunch get injected after the first bunch completely dephased. This bunch was accelerated to .8GeV. These results were published in Phys. Rev. Lett. [Tsung:2004]. Subsequent to the submission date three separate laboratories carried out experiments in which mono-energetic electron beams were observed. The experimental results were all published a single issue of Nature [we were co-authors on one, Mangles:2004]. Although the parameters varied, 3D PIC simulations of each experiment showed that these beams arose from similar physics to what we reported in the Phys.Rev.Lett. F.S.Tsung gave an invited talk at the 2005 DPP Meeting on this topic [Tsung:2006].

Subsequently, we have continued to use OSIRIS to model ongoing LWFA experiments throughout the world. These simulations were critical to the development of the first phenomenological theory of LWFA in the nonlinear blowout regime [Lu:2007]. An example of these simulations is shown in figure 4. Additionally, simulations using OSIRIS were an important part of a collaboration between Imperial College, Rutherford Appleton Laboratory (RAL), and UCLA. The simulations modelled experiments carried out at the Central Laser Facility of RAL as well as several other laser labs in Europe. These simulations helped explain many experimental observations, such as the pattern of synchrotron radiation from electrons accelerated in a Petawatt laser generated plasma cavity[Kneip:2008], the effect of laser focusing conditions on propagation [Thomas:2007], monoenergetic electron production in laser wakefield accelerators [Mangles:2004], the generation of collimated multi-MeV ion beams from high intensity laser interactions with underdense plasma[Willingale:2006], and experimental evidence of laser wakefield acceleration of monoenergetic electron beams in the first plasma wave period [Mangles:2006]. Together with our collaborators at IST in Portugal, we have also modelled parameters for a planned upgrade at RAL to 300J in 30fs (see proposed work section). We also simulated a successful experiment carried out at UCLA which showed cm scale self-guiding of ultra-short laser pulse in low density plasmas [Ralph:2008]. This experiment was motivated by our new phenomenological theory on of LWFA in the blowout regime, in which it is found that self-guiding of ultra-short laser pulses over a significant fraction of the pump depletion distance is possible. Both the experimental and 3D full-scale PIC simulation results indicate that self-guiding is effective for laser powers as low as the critical power for relativistic self-focusing, P_C , in the density range $5\text{-}7 \times 10^{18} \text{cm}^{-3}$.

Figure 4: On the left, energy spectra of a 10fs 1.5GeV monoenergetic electron beam created in the blowout regime of LWFA from a lab frame 3D PIC simulation using OSIRIS. On the right, energy spectra obtained for the same physical condition from a 3D PIC simulation in a Lorentz boosted frame using OSIRIS.

E. Petawatt laser-plasma interactions:

In collaboration with Imperial College and RAL, we modeled experiments carried out at the Vulcan Petawatt facility at the Rutherford Appleton Laboratory (RAL). In these experiments a 650fs, 1mm, 160 J laser is focused onto a gas jet. The resulting plasma density ranges from 10^{19} to 10^{20} cm^{-3} with an axial length of $\sim 2\text{mm}$. These experiments observed 10 MeV ions expelled radially as well as 300 MeV electrons in the forward direction. Using OSIRIS, it was determined that the ions arise from an ion acoustic shock driven by the transverse ponderomotive force [Willingale:2006]. The energetic electrons appear to arise from a combination of stochastic and betatron resonance effects. Using particle tracking diagnostics, we determined that the energy comes almost exclusively from the component of the electric field transverse to the laser propagation direction. When the PW class laser propagates through the underdense plasma it expels plasma electrons radially. The resulting space charge pulls the ions out creating the shocks. Residual electrons left in the channel experience both the fields of the laser and that of the ion column. Others have shown that a betatron resonance is possible between the oscillations in the laser field and in the ion channel. However, it is not straightforward for electrons to come into resonance, particularly for very tenuous plasmas. We find that electrons are stochastically accelerated up to an energy at which they can get into a betatron resonance [Mangles:2005].

F. Development of a theory for wakefield excitation in the blowout regime:

We studied in great detail the wakes excited by intense particle beams. We examined how and when linear fluid theory breaks down. This work was published in Phys. Plasmas. We also developed a theory for nonlinear, multi-dimensional plasma waves with phase velocities near the speed of light. This theory is appropriate for describing plasma waves excited when all electrons are expelled from a finite region by either the space charge of an intense particle beam or the radiation pressure or an intense laser. It makes connection to linear fluid theory results and works very well for the first bucket before phase mixing occurs for very nonlinear wakes. We separate the plasma response into a cavity or blowout region void of all electrons and a sheath of electrons just beyond the cavity. This is illustrated in figs. 5a and 5b where the blowout radius is defined in fig. 5a. Although there is considerable trajectory crossing the details can be incorporated into a simple model for the sheath as described in fig. 5b. This simple model permits the

derivation of a single equation for the boundary of the cavity, i.e., the blowout radius, $r_b(\xi)$. In fig. 5 we plot solutions to our equation for $r_b(\xi)$ as well as results from PIC simulations. The results are indistinguishable. This model describes the structure of both the accelerating and focusing fields in a relativistic, multi-dimensional plasma wave. The accelerating field within the cavity is given by $\frac{eE_z}{mc\omega_p} \equiv \varepsilon = \frac{k_p r_b(\xi)}{2} \frac{dr_b(\xi)}{d\xi}$. In these multi-dimensional wakes, there are both longitudinal and radial E fields as well as azimuthal magnetic fields. When the maximum radius, $r_{b\max}$, of the of the cavity or ion column is much greater than a collisionless skin depth then the cavity has a spherical shape and the accelerating field has linear slope of $\varepsilon = \xi/2$ where $\xi = z - ct$. Therefore, the peak accelerating field $\varepsilon_{\max} = r_{b\max}/2$. While others have begun to analyze these nonlinear wakes in special limits, this is the first predictive theory. This work was published to Physical Review Letters [Lu:2006a] and to Physics of Plasmas [Lu:2006b]. The graduate student, W.Lu, who did this work gave an invited talk on this topic at the 2005 DPP meeting in Denver.

Figure 5: a) The beam (red) and plasma density from a simulation of wake excitation in the blowout regime. The definition of $r_b(\xi)$ is given and the sheath (green) is seen. b) A lineout in radius of the plasma density minus the normalized current. The red curve is from the simulation while the blue is the model profile we use in our theory. c) Trajectories for $r_b(\xi)$ from our theory compared against PIC simulation results. In each case the curves fall on top of each other.

F. Development of a Phenomenological framework of LWFA in the blowout regime and relevant full scale 3D explicit and reduced model PIC simulations:

We developed the first phenomenological theoretical framework of LWFA in the blowout regime [Lu:2007]. In this framework, we identified and described the key physical mechanisms of laser wakefield acceleration (LWFA) in the blowout or “bubble” regime: these included appropriately matching the laser intensity, spot size, and pulse length for the plasma density, nonlinear wakes in the blowout regime, local pump depletion (photon deceleration), dephasing, self-guiding or matched channel guiding, beam loading, and self-injection. Based on these concepts, we derived the design formulas for achieving stable acceleration for a LWFA stage. We also systematically used very large scale 3D parallel PIC simulations to verify these formulas and very good agreement was achieved. We used fully explicit OSIRIS simulations in both lab frame and a Lorentz boosted frame and QuickPIC simulations of channel guided LWFA. Some highlights were: (1) a 0.3nC, 10fs, 1.5GeV electron bunch produced by a 30fs 200TW laser interacting with a 0.75cm long plasma with a density $1.5 \times 10^{18} \text{cm}^{-3}$ (simulations are

done in both lab frame and a Lorentz boosted frame). (2) a 4nC, 12GeV electron bunch produced by a 110fs 300J laser interacting with a 22cm long plasma with a density $2.7 \times 10^{17} \text{cm}^{-3}$ (in a Lorentz boosted frame). (3) 3D QuickPIC simulations of .5-100GeV matched channel-guided LWFA (see figure 6).

Figure 6: On the left, the energy spectral (0.5-100GeV) from QuickPIC simulations of LWFA in a matched plasma channel for different peak laser powers and plasma densities. On the right, plots of the plasma densities (2D slices) for a 10GeV QuickPIC simulation at different laser propagation distances, which show a very stable wake structure over long distance.

G. Development of a theory for electron hosing instability in the blowout regime:

One of the biggest obstacles for LWFA and PFWA is hosing (In both the trailing beam can hose and in the PFWA the drive beam can also hose). Hosing is an instability which is due to a coupling between the centroid of the beam and the ion channel (focusing force on the beam). Hosing could lower the overall efficiency by breaking the drive beam apart before it propagates a sufficient distance. It could also greatly distort the accelerating field such that the trailing beam will acquire a large energy spread. It also leads to a sloshing of the trailing beam making it difficult to align and collide two beams. We recently developed a theory [Huang:2007] for the hosing of short-bunches that relies heavily on the insight obtained from QuickPIC simulations and our theory for wake excitation in the blowout regime (that was mostly developed during the previous grant period). Previous hosing theory only considered the adiabatic (long pulse) & non-relativistic regime. We extended the theoretical analysis to three other regimes, namely adiabatic & relativistic, non-adiabatic & non-relativistic, and non-adiabatic & relativistic. Through QuickPIC simulations, we find our theory gives very accurate predictions for the hosing growth and that the growth rate for short, intense bunches is reduced because the blowout radius is larger (by at least a factor of 2) from the equilibrium radius of long bunches, because of relativistic mass increases, and because of the axial motion of electrons in the sheath. On the left of figure 7, we plot the plasma and beam density in a x-z slice. In the middle we plot the evolution of the beam centroid vs. propagation distance for a location near the center of the beam. The blue curve is the old theory and the red curve is the simulation result. The new theory curves lie very close to the red curve.

Figure 7: Left: A 2D electron density slice from a QuickPIC simulation, which shows the hosing of a short beam. Middle: Plots of hosing growth from old theory (blue) and new theory (red). Simulation data (in other colors) is on top of red. Right: Electron density plot and the lineout of wakefield from an OSIRIS simulation for a properly shaped trailing bunch that flattens the wakefield.

H. Development of a theory for nonlinear beam loading in the blowout regime:

The topic of beam loading involves determining the optimal shape and placement of the trailing beam within the wakefield which most efficiently transfers energy from the wake to the trailing beam. The compromise is acceleration gradient versus the beam charge. In addition, one wants to maintain beam quality. There has been little work in this area since the seminal work of Katsouleas et al. in which they used linear superposition to calculate how loading particles modifies the wake. Based on our theory for wake excitation in the blowout regime [Lu:2005][Lu:2006][Lu:2006:2], we derived theory for beam loading in this nonlinear regime where linear superposition cannot work. Analytical solutions for the fields and the shape of the ion channel are derived and published in Physical Review Letters [Tzoufras:2008]. It was shown that very high beam-loading efficiency can be achieved, while the energy spread of the bunch can be minimized by choosing a proper bunch shape. On the right-hand-side of figure 7, we show how a properly shaped (inverse trapezoid) trailing bunch can flatten the wakefield. A flattened wakefield leads to little energy spread.

E. Successful implementation of the Lorentz boosted frame concept for LWFA:

In collaboration with IST in Portugal, we have developed the capability to model LWFA in a Lorentz boosted frame. To our knowledge we are the first to do so in 3D. Recently, motivated by beam-plasma interactions in accelerators and FEL's, J.-L. Vay showed that although the physics conclusions do not change from one frame to another, the computational requirements can in principle be significantly different. For LWFA the idea is that in the lab frame (and using the moving window) the laser wavelength is very short compared to the laser propagation distance. On the other hand in a frame moving with the wake, the laser and wake wavelengths are elongated by 2γ , while the plasmas length is Lorentz contracted by γ . The box size must be g times longer in physical units however the number of cells is the same since now the laser wavelength is also elongated

(the number of laser cycles is an invariant). However, the plasma is shorted by γ so the number of time steps is correspondingly less. In addition, the time step, which is set by the cell size divided by the speed of light, is reduced. In a 1D calculation this reduction would be another factor of γ , leading to a potential savings $\sim \gamma^2$. However, in multi-dimensions the time set by the larger of the cell size for each dimension, so the actual savings is less. For practical reasons γ is less than γ_f .

The fundamental code algorithm needs no change, but running the simulation in a different frame poses particular numerical difficulties. The first is related to the relativistic velocity of the plasma in the boosted frame, which can lead to numerical noise due to the accumulation of round-off errors when adding the current of background electrons and ions. Improving the grid deposition method with the use of different arrays for each species is a possible solution for this noise. A second issue is electromagnetic waves that propagate backwards. In figure 4 we show results from OSIRIS simulations in the lab and boosted frame for a case taken from our recent publication on a phenomenological theory [Lu:2007]. The boosted frame simulation required ~ 30 times few CPU hours. [Martins:2008]. In figure 8 (left) we show results from boosted frame simulations for parameters that cannot yet be modeled in the lab frame due to lack of the necessary computing resources. In figure 8 (right) is an example of a more nonlinear case from the lab frame to contrast it with the case in figure 8 (left).

Figure 3: Comparison of electron density and electron energy phase space between a low density and a high plasma density 3D PIC simulations for a 300J laser. Left: The plasma density is chosen as $2.7 \cdot 10^{17} \text{cm}^{-3}$ and laser pulse length is 110fs (Simulation is done in a Lorentz boosted frame). Right: The plasma density is $1.5 \cdot 10^{19} \text{cm}^{-3}$ and laser pulse length is 30fs (simulation is done in lab frame).

G. Construction of DAWSON:

We were awarded an NSF MRI award to build a 512 processor cluster. The PI for the NSF MRI is the PI for this proposal. **There are substantial university resources being devoted to managing this cluster.** In addition, to providing the staff that manages it, the university provides space in an air-conditioned environment (it weighs 5 tons and produces 250000 BTU's of heat per hour). The cluster was constructed a year ahead of schedule and has been very stable. Much of the simulation results presented in this

proposal were done on this machine. Details of the cluster, called DAWSON, can be found in the facilities section.

List of relevant publications:

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