Speed optimal implementation of a fully relativistic 3d particle push with charge conserving current accumulation on modern processors

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On modern processors, the floating-point subsystem performance far exceeds that of the memory subsystem such that traditional vector oriented implementations of particle-in-cell methods can only attain a small fraction of the theoretical performance. Building on prior work [1], a highly optimized fully relativistic 3d particle push / accumulate has been implemented. The push uses the standard leap-frog particle advance with a 6^{th} order accurate Boris rotation (the same as [2]). The field interpolation and the charge conserving current accumulation are implemented according to the prescription in [3]. The data structures used allow for very flexible partitioning strategies and variably weighted particles.

The implementation has been carefully designed to minimize memory traffic between main memory and the processor, minimize cache thrashing, maximize the locality of memory accesses and to allow SIMD extensions present on modern processors to be taken advantage portably. At the time of this writing, a particle advance of 6 million particles pushed and accumulated per second has been achieved in the common case on an AMD Athlon workstation with a 1.733GHz processor and DDR266 DRAM memory subsystem. This can be shown to be near the theoretical workstation performance.

Some of the characteristics of modern processors and methods used to optimally implement the above particle advance on them will be discussed.

[1] Bowers. "Accelerating a Particle-In-Cell Simulation Using a Hybrid Counting Sort." *Journal of Computational Physics.* 173. 393-411. 2001.
[2] Blahovec *et al.* "3-D ICEPIC simulations of the relativistic klystron oscillator." *IEEE Transactions on Plasma Science.* 28. 821. 2000.
[3] Eastwood *et al.* "Body-fitted electromagnetic PIC software for use on parallel computers." *Computer Physics Communications.* 87. 155-178. 1995.