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PIC for Accelerator Science

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Fermilab

For the ComPASS Collaboration

The ComPASS Collaboration

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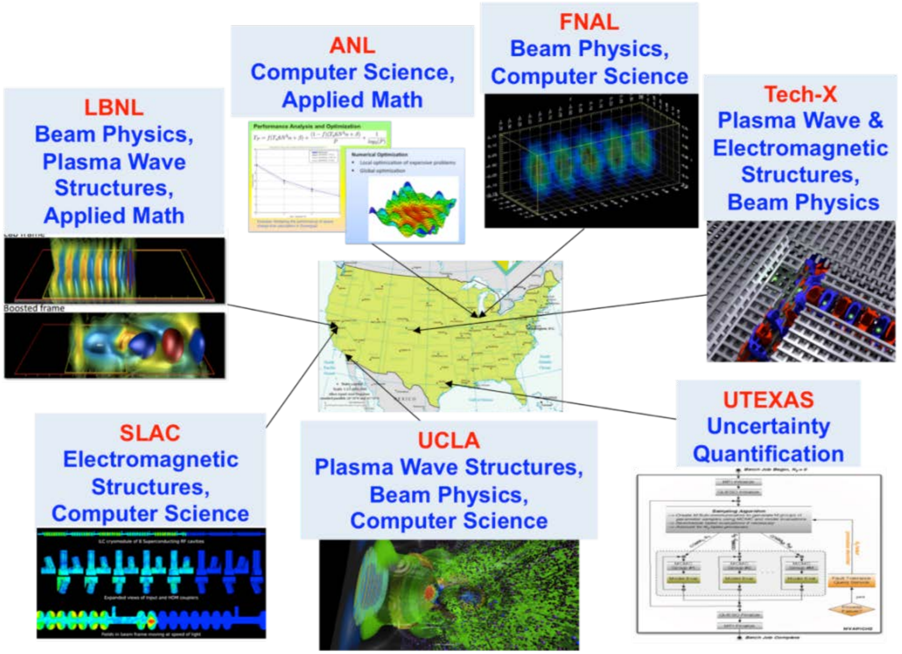
Community Project for Accelerator Science and Simulation

- To enable scientific discovery in HEP, high-fidelity simulations are necessary to develop new designs, concepts and technologies for particle accelerators
- Under SciDAC3, ComPASS is developing and deploying state-of-the-art accelerator modeling tools that utilize
  - the most advanced algorithms on the latest most powerful supercomputers
  - cutting-edge non-linear parameter optimization and uncertainty quantification methods.



This talk

- PIC methods
- Two closely related application areas
  - Beam Dynamics
  - Advanced Accelerators
  - Require tracking particles interacting with fields calculated on grids
- HEP (Fermilab, UCLA) working with ASCR [FastMATH (LBNL), Fermilab, UCLA]
- Only one sub-topic of the ComPASS project. For a comprehensive overview, see SciDAC PI 2012 talk by Panagiotis Spentzouris

Application areas: Beam Dynamics and Advanced Accelerators

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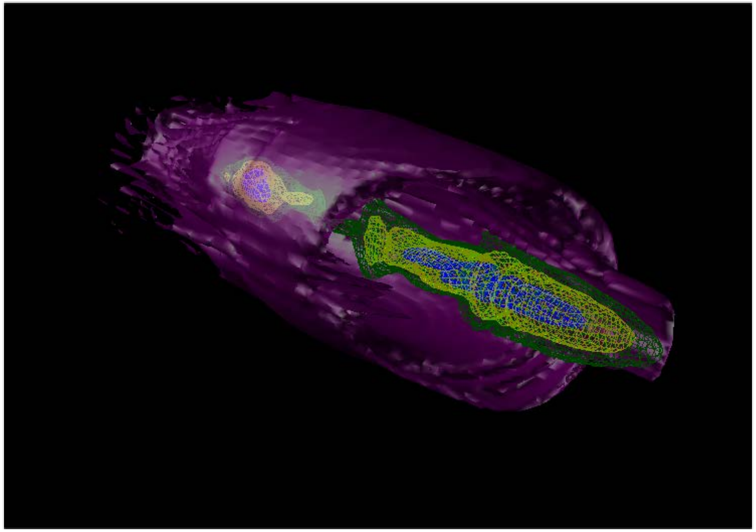
- Beam Dynamics
  - Existing and planned accelerators
  - Complex devices that need to be simulated for long times
    - Accelerators can have 1000s of elements
    - 1000s to 1000000s of revolutions

- Advanced Accelerators
  - Next-generation acceleration technology
    - Huge field gradients promise dramatically smaller/cheaper accelerators
    - Two types
      - Plasma-wakefield acceleration (PWFA)
      - Laser-wakefield acceleration (LWFA)
  - Complex fields, short time scales



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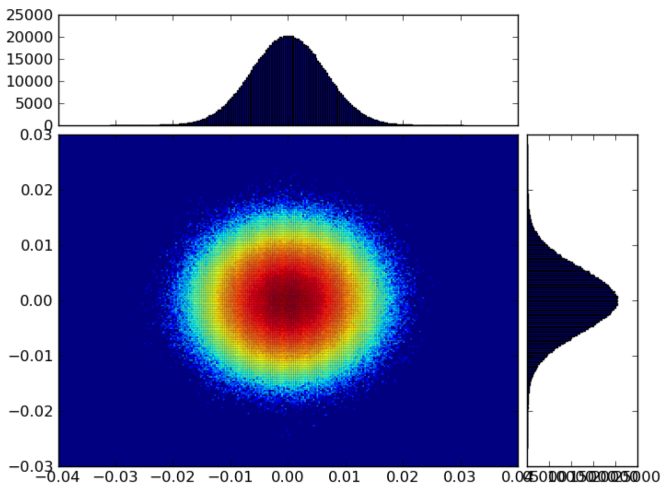
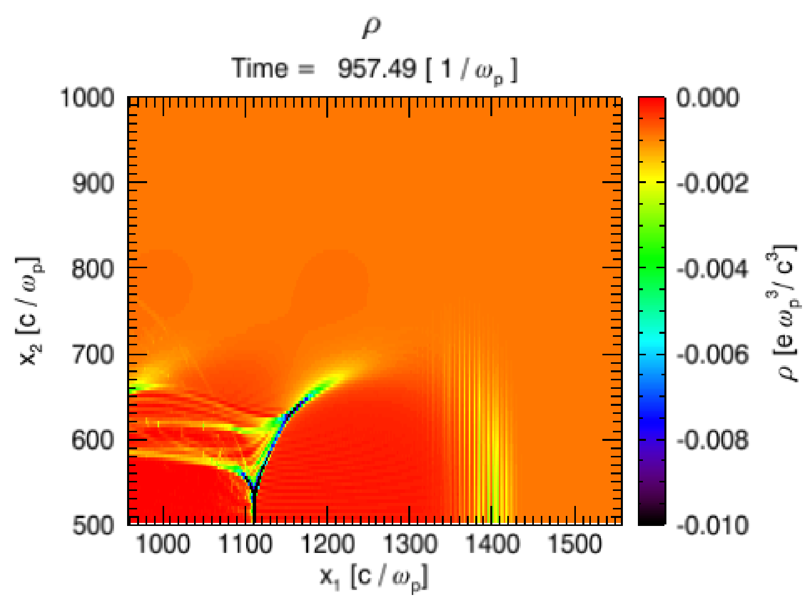
Application areas: Beam Dynamics and Advanced Accelerators

- Beam Dynamics
  - Internal + External fields
    - External field calculations trivially parallelizable
      - All P, no IC
    - Internal field calculations same as AA
  - Minimal bunch/field structure



- Advanced Accelerators
  - Pure PIC
  - Complicated bunch/field structure



Scaling achievements to date in beam dynamics and advanced accelerators

Beam Dynamics: scaling achievements

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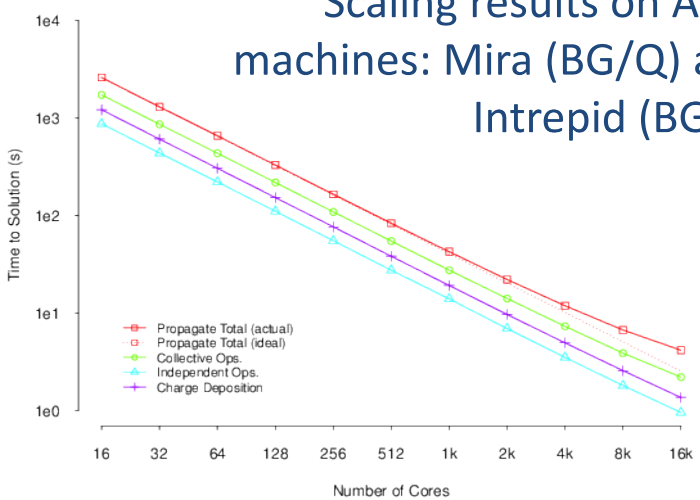
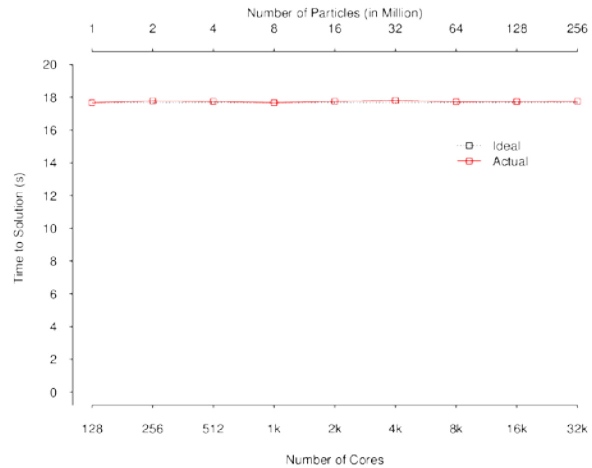
- Synergia
  - Single- and multiple-bunch simulations

Scaling results on ALCF machines: Mira (BG/Q) and Intrepid (BG/P)

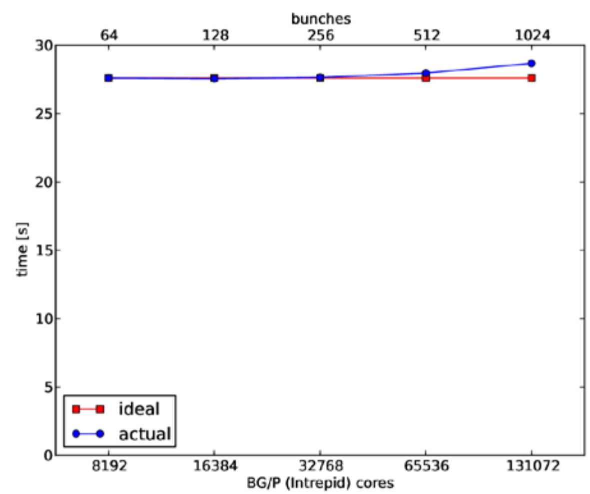


Single-bunch strong scaling from 16 to 16,384 cores

32x32x1024 grid, 105M particles



Weak scaling from 1M to 256M *particles* 128 to 32,768 cores



Weak scaling from 64 to 1024 *bunches*

8192 to 131,072 cores

Up to over 10^{10} particles

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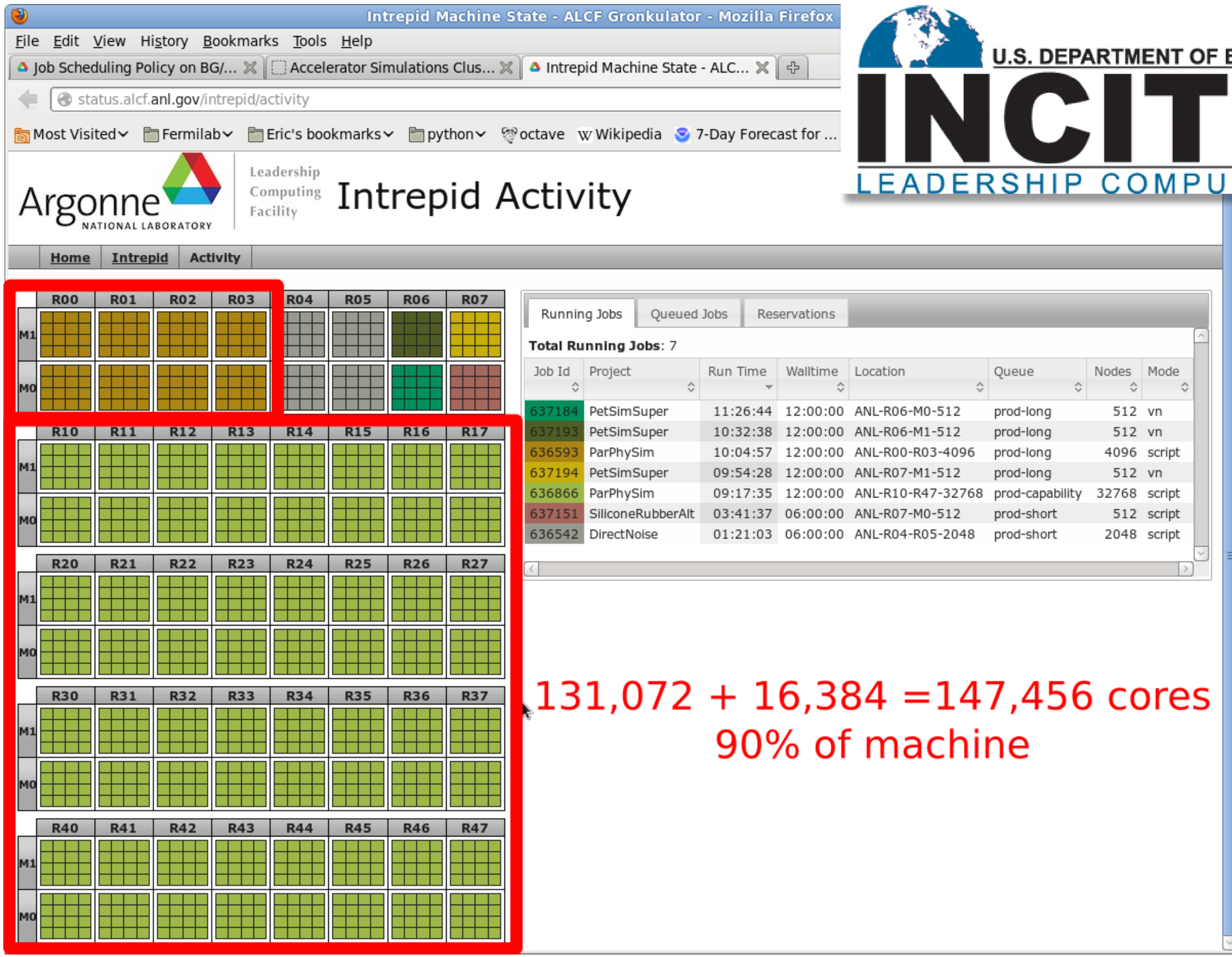
Synergia in production



Job Id	Project	Run Time	Walltime	Location	Queue	Nodes	Mode
637184	PetSimSuper	11:26:44	12:00:00	ANL-R06-M0-512	prod-long	512	vn
637193	PetSimSuper	10:32:38	12:00:00	ANL-R06-M1-512	prod-long	512	vn
636593	ParPhySim	10:04:57	12:00:00	ANL-R00-R03-4096	prod-long	4096	script
637194	PetSimSuper	09:54:28	12:00:00	ANL-R07-M1-512	prod-long	512	vn
636866	ParPhySim	09:17:35	12:00:00	ANL-R10-R47-32768	prod-capability	32768	script
637151	SiliconeRubberAlt	03:41:37	06:00:00	ANL-R07-M0-512	prod-short	512	script
636542	DirectNoise	01:21:03	06:00:00	ANL-R04-R05-2048	prod-short	2048	script

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

131,072 + 16,384 =147,456 cores
90% of machine

Advanced Accelerators: scaling achievements

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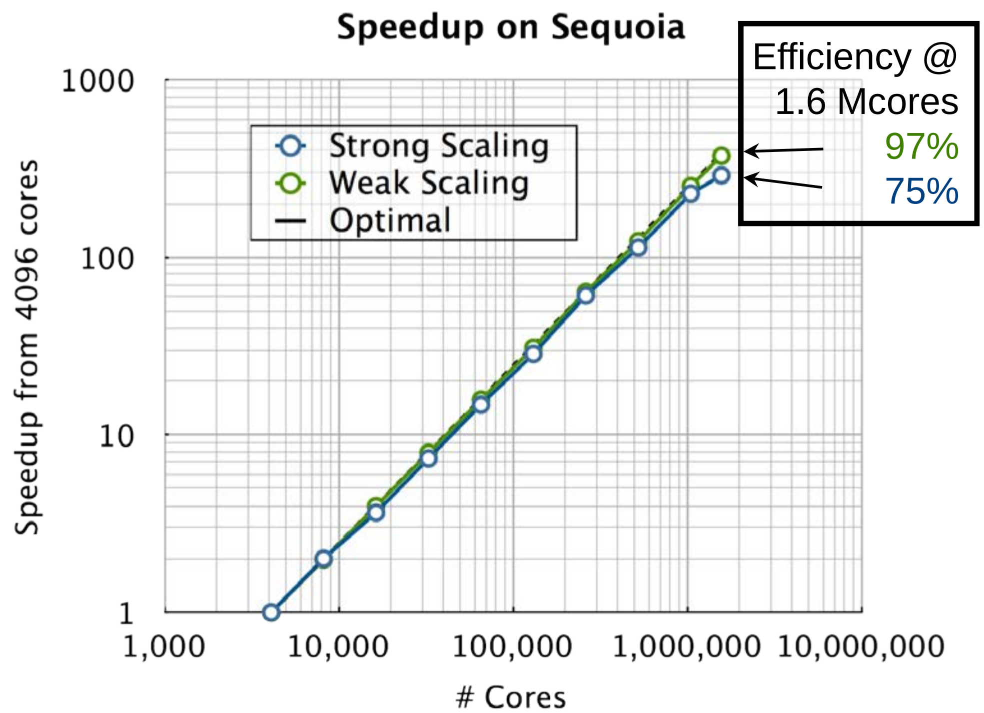
OSIRIS: 1.6 million cores and 2.2 PFLOPS

- Performance tests on Blue Waters
  772 480 cores (XE partition)
- Problem size
  cells = 38624 × 1024 × 640
  400 particles/cell (~ 10^{13})
- Computations
  2.2 PFlop/s performance
  31% of R_{peak}

UCLA



How we achieved scaling in Synergia

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- Challenge: beam dynamics simulations are big problems requiring many small solves
  - Typically $64^3 - 128^3$ (2e5 – 2e6 degrees of freedom)
    - Compare with 2.5e10 in OSIRIS scaling benchmark
  - Will never scale to 1e6 cores
  - Need to do many time steps (1e5 to 1e8)
- All "scaling" advice we received was with respect to grid size
  - Included decomposing particles by grid location
  - In beam dynamics, external fields can cause particles to move over many grid cells in a single step
    - Communication required to maintain decomposition and load balancing
      - Point-to-point communication
      - Complicated for both programmer and end user
        - » Change in physical parameters can change communication time by x100

Synergia: first scaling advances

- Eliminate particle decomposition
  - Requires collective communication
    - But not point-to-point
    - Big machines are optimized for collectives
  - Simpler for programmer and end-user
  - Helps a little, but leads to…
- Breakthrough: Redundant field solves (communication avoidance)
  - Field solves are a fixed-size problem
    - Scale to $1/n^{th}$ of problem

Synergia: communication avoidance

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- Communication avoidance
  - Used to have two global communications
    - collect charge density
    - broadcast calculated field (x3 dimensions)
  - Fields are now limited to a small set of cores, so the latter is greatly reduced
- Allows scaling in number of particles
  - Not limited by the scalability of the field solves
  - Excellent (i.e., easy) scaling

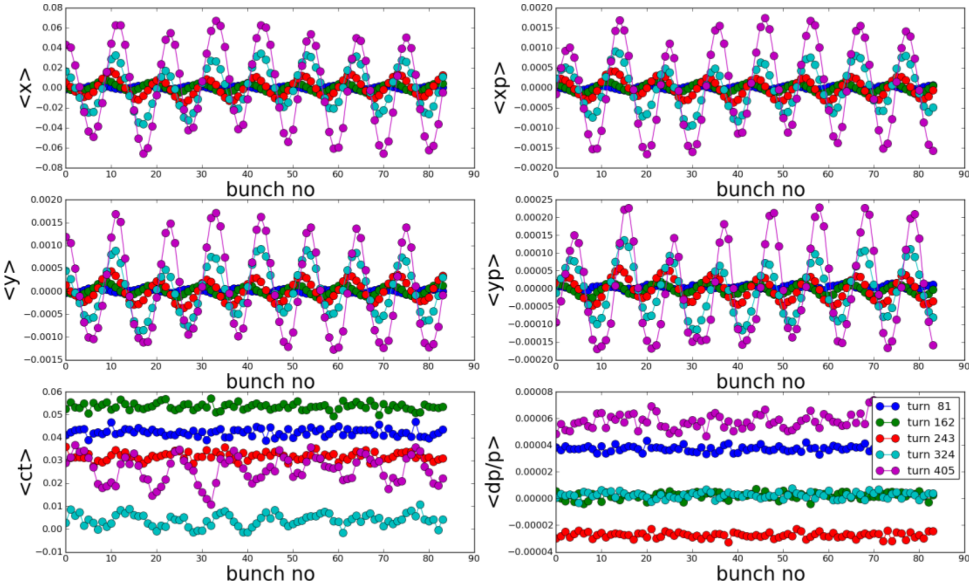
Synergia: large numbers of particles

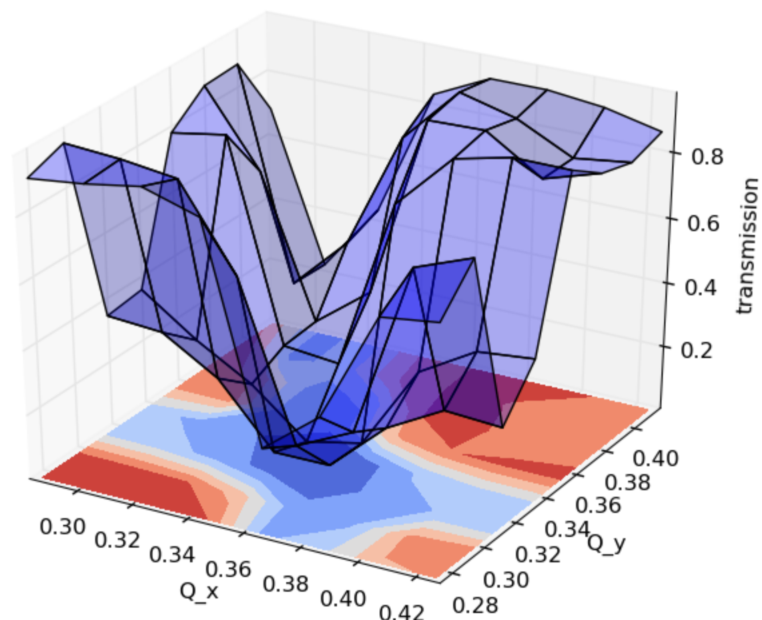
- Many reasons to use more particles and/or more complex particle calculations
  - Accuracy of long-term simulations
    - Statistical errors in field calculations become more important as the number of steps increases
  - Detailed external field calculations
    - Significant feature of Synergia
    - Application-dependent
  - Accurate calculation of small losses
    - High-intensity accelerators require very small losses
      - Calculating 1e-5 losses at 1% requires 1e9 particles

Synergia: new scaling opportunities

- Multi-bunch wakefield calculations
  - Excellent scaling
    - Bunch-to-bunch communications scale as O(1)
      - Also relatively small
  - Already discovered multi-bunch instabilities in the Fermilab Booster
    - Not accessible with “fake” multi-bunch

- Parallel sub-jobs
  - Parameter scans, optimization
  - Part of our workflow system
    - Makes it easier on end user
    - Avoids error-prone end user editing of job scripts





Synergia: scaling final

- Scaling advances are the product of many factors
  - Redundant solves (communication avoidance) (x4-x10)
    - Every simulation
  - Large statistics (x1-x1000)
    - Some simulations
  - Multiple bunches (x1-x1000)
    - Some simulations
  - Parallel sub-jobs (x1 – x100)
    - Some simulations
- Product can be huge (x4 – x1e8)

GPUs and multicore architectures

Emerging technology research

- GPUs and Multicore
  - Shared memory is back!
  - Some things get easier, some harder
    - Charge deposition in shared memory systems is the key challenge
- Multi-level parallelism very compatible with our communication avoidance approach

Advanced Accelerator simulations on GPUs and multicore

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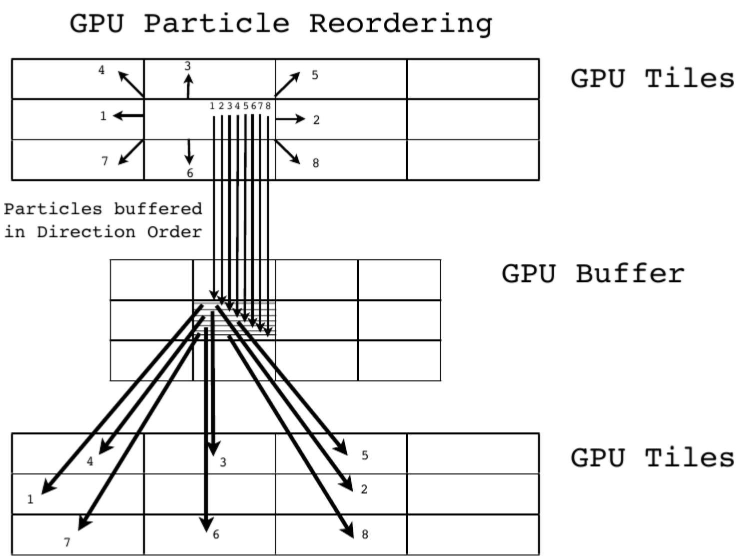
V. Decyk and T. Singh

- We have developed an algorithm for GPUs which gives good performance and appears to be portable to other emerging architectures.
- It is based on dividing space into small tiles and requires a fast particle reordering scheme which is called every time step.
- Currently runs on NVIDIA GPUs and OpenMP multi-core processors. Should run on Intel PHI.
- Different architectures require different implementations, but data structures are largely the same, and code can be recompiled with different libraries on different architectures.
- 2D Electrostatic and 2-1/2D Electromagnetic codes run on one GPU. 2D Electrostatic on multiple GPUs with MPI.
- Skeleton codes will be made available on the UCLA IDRE web site:
  - https://idre.ucla.edu/hpc/parallel-plasma-pic-codes



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AA: GPU-accelerated results

- Benchmark with 2048x2048 grid, 150,994,944 particles, 36 particles/cell
- optimal block size = 128, optimal tile size = 16x16. Single precision
- GPU algorithm also implemented in OpenMP

- Electrostatic
- mx=16, my=16, dt=0.1
- Total speedup was about 35 compared to 1 CPU, and about 3 compared to 12 CPUs.

	CPU:Inteli7	GPU:M2090	OpenMP(12 cores)
Push	22.1 ns	0.532 ns	1.678 ns
Deposit	8.5 ns	0.227 ns	0.818 ns
Reorder	0.4 ns	0.115 ns	0.113 ns
Total Particle	31.0 ns	0.874 ns	2.608 ns

- Electromagnetic
- mx=16, my=16, dt=0.04, c/vth=10
- Total speedup was about 51 compared to 1 CPU, and about 4 compared to 12 CPUs.

	CPU:Inteli7	GPU:M2090	OpenMP (12 cores)
Push	66.5 ns	0.426 ns	5.645 ns
Deposit	36.7 ns	0.918 ns	3.362 ns
Reorder	0.4 ns	0.698 ns	0.056 ns
Total Particle	103.6 ns	2.042 ns	9.062 ns

Beam dynamics simulations on GPUs and multicore

Fermilab Q. Lu, JFA

- *Nearly* the same problem as in AA
  - Particles can move many cells in between steps
- Optimal decomposition/deposition schemes differ

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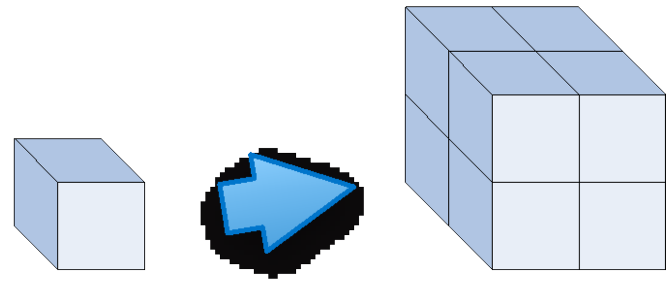
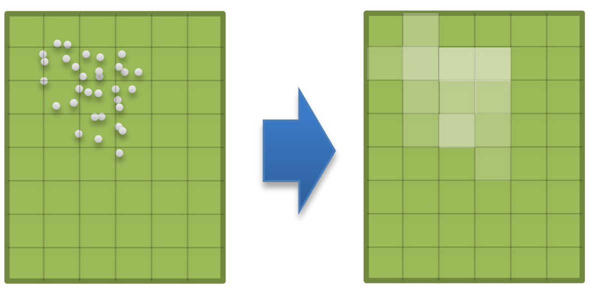
Charge deposition in shared memory

One macro particle contributes up to 8 grid cells in a 3D regular grid





Collaborative updating in shared memory needs proper synchronization or critical region protection

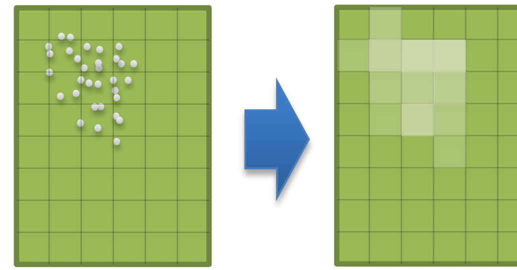
CUDA

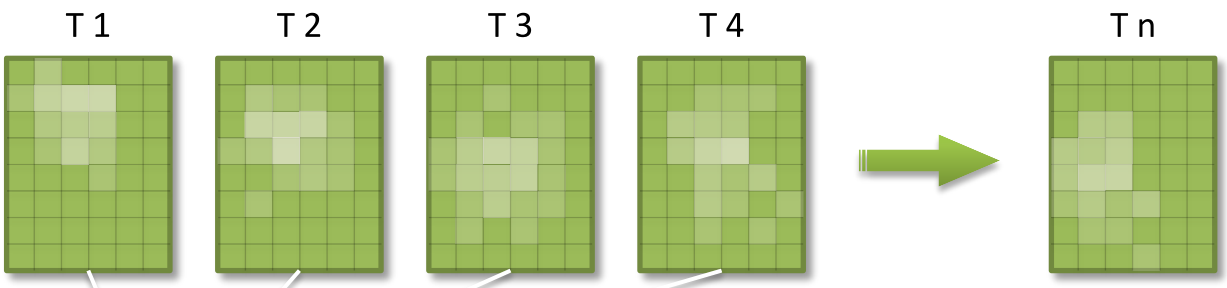
- No mutex, no lock, no global sync
- Atomic add – yes, but not for double precision types

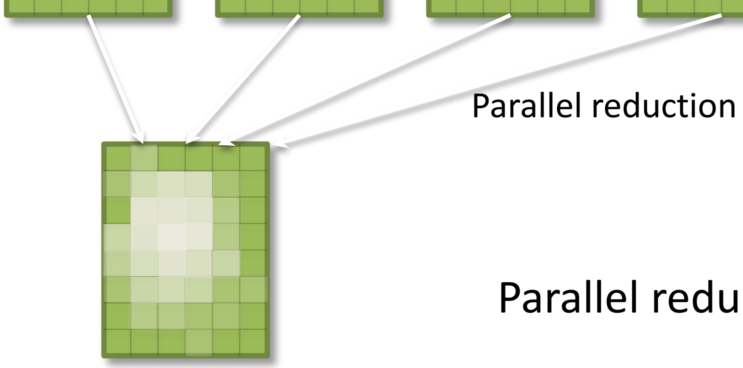
OpenMP

- ***#pragma omp*** critical
- ***#pragma omp atomic***
- ***Both very slow***

Charge deposition in shared memory – solution 1







Each thread has a duplicated spatial grid, and charges will be deposited to that grid only

Parallel reduction among all n-copy of spatial grids

CUDA

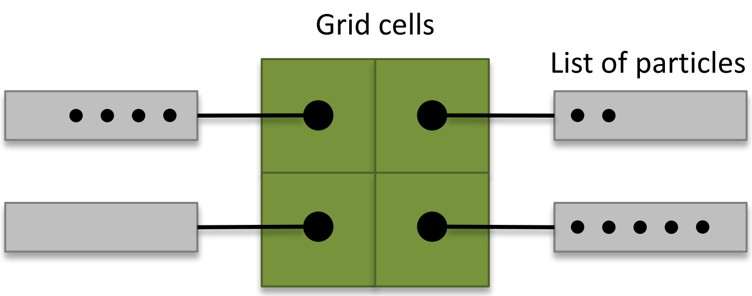
- Concurrency be an issue for GPU
- Memory bottleneck at final reduction

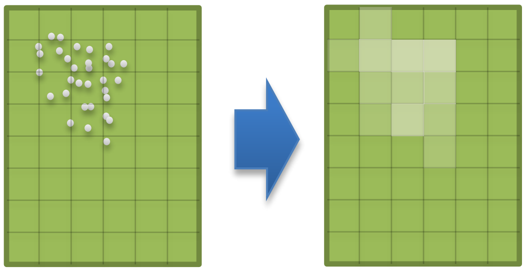
OpenMP

- Works well at 4 or 8 threads
- Scales poorly at higher thread counts

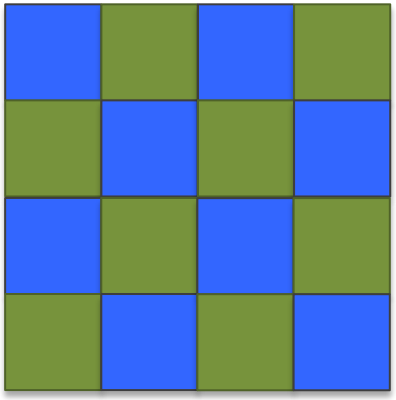
Charge deposition in shared memory – solution 2

Sort particles into their corresponding cells using parallel bucket sort





Deposit based on color-coded cells in an interleaved pattern (red-black)



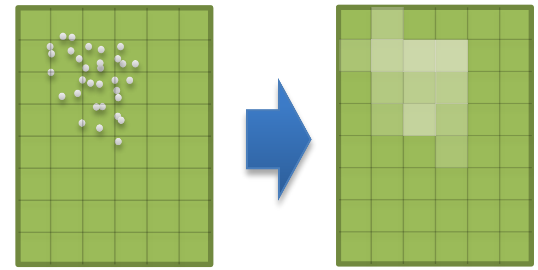
CUDA

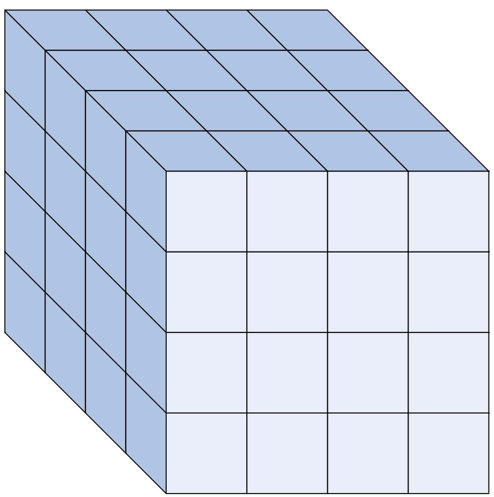
- High thread concurrency
- Good scalability, even the overhead shows reasonable scaling
- No memory bottleneck
- Better data locality at pushing particles

OpenMP

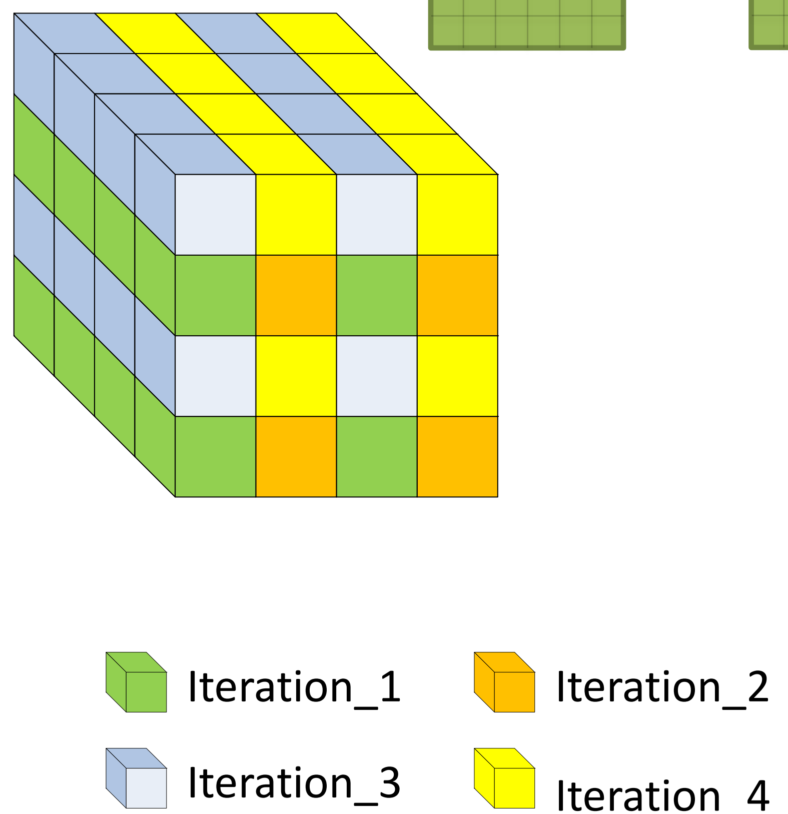
- Non-trivial sorting overhead for low thread counts

Charge deposition in shared memory – solution 2

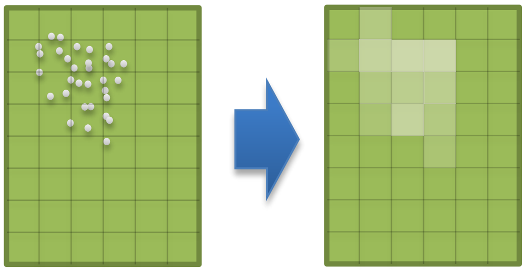




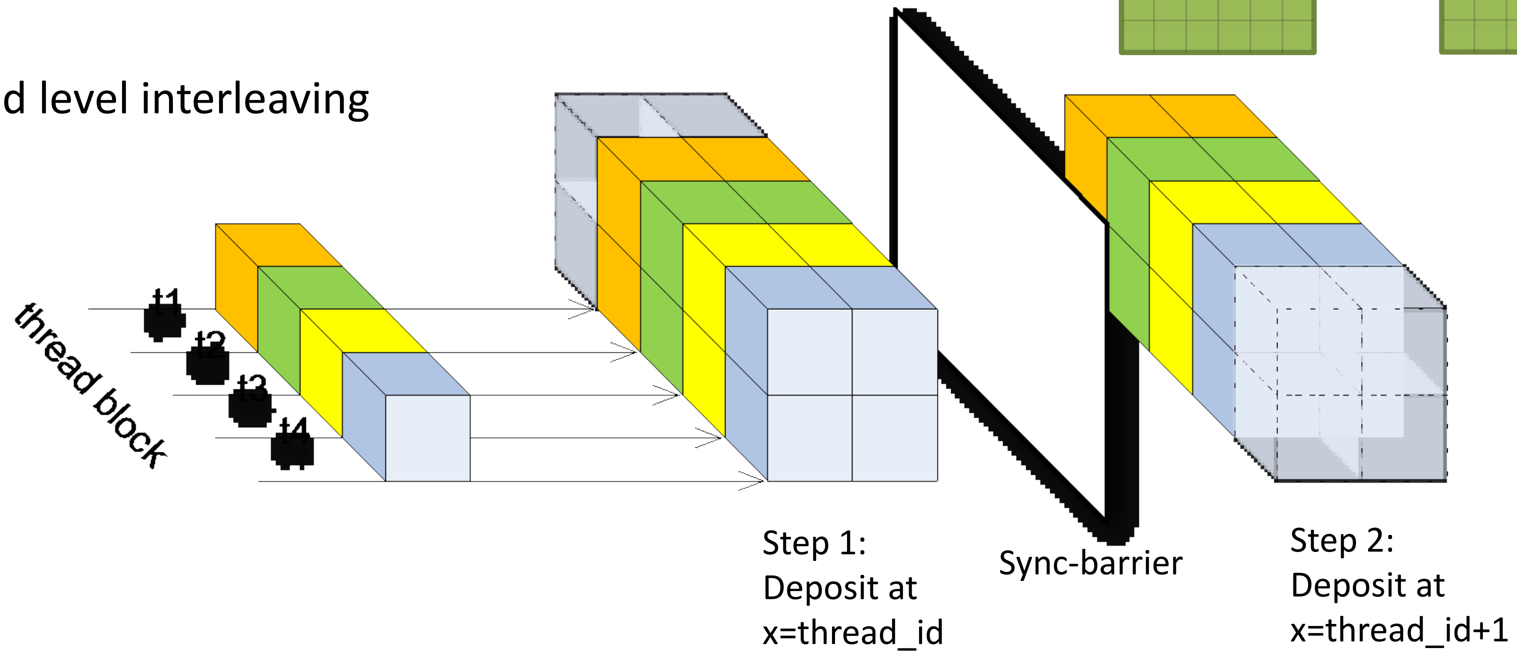
Grid level interleaving

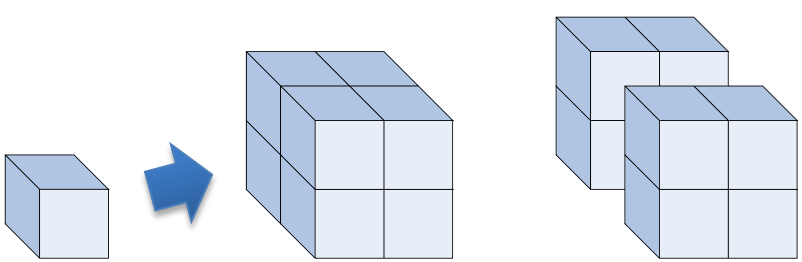


Charge deposition in shared memory – solution 2



Thread level interleaving





BD: GPU and multicore results

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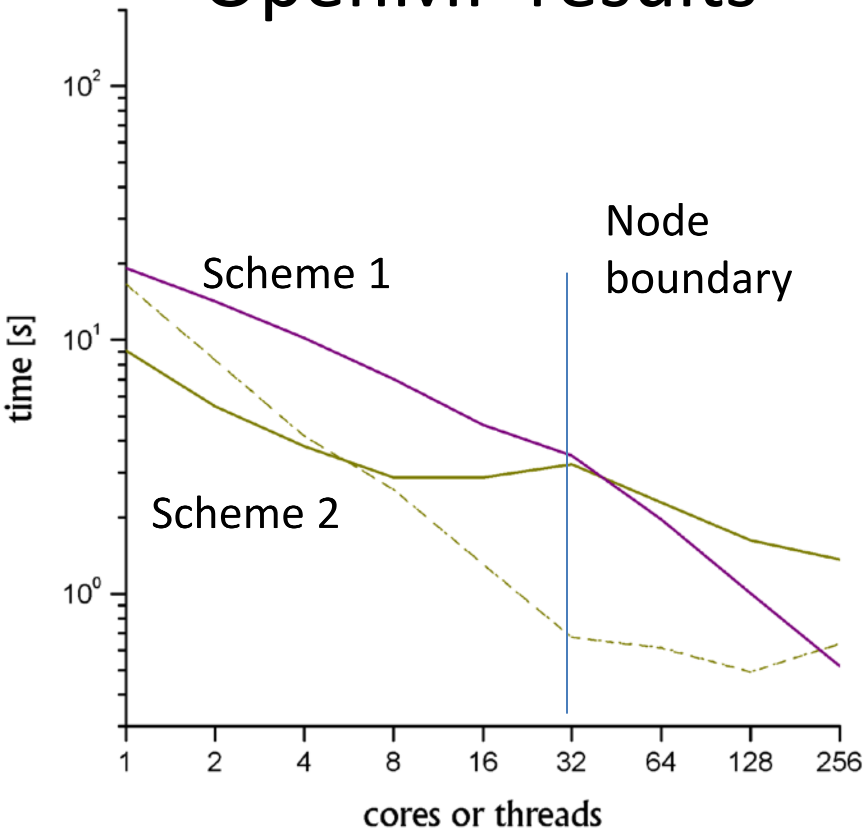
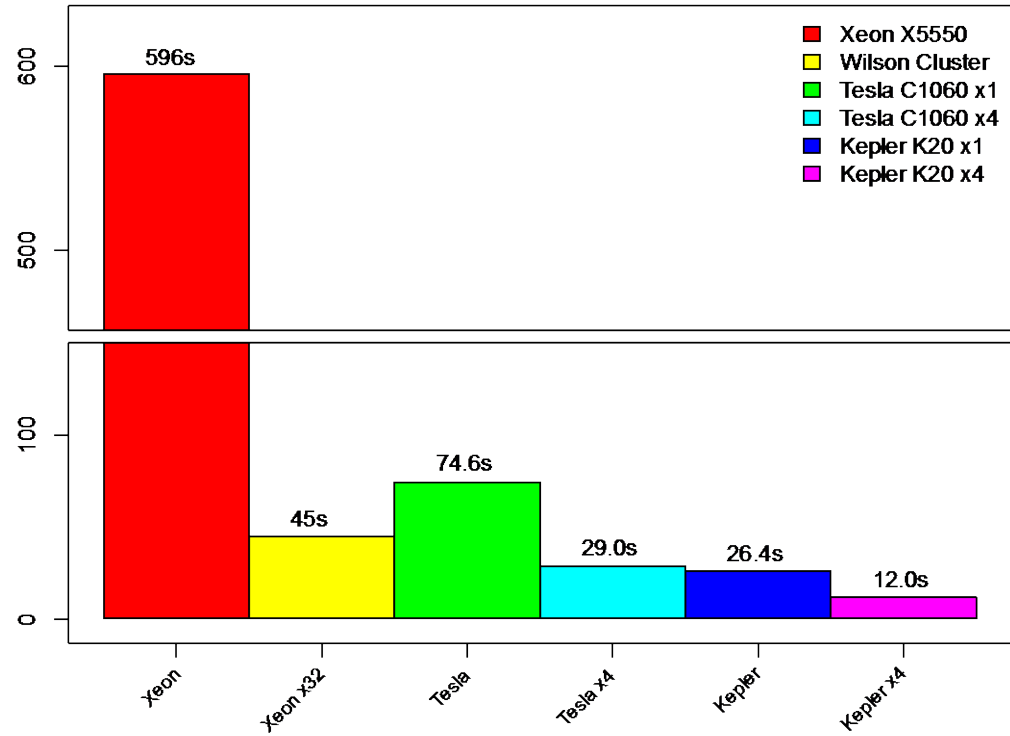
OpenMP results



GPU results



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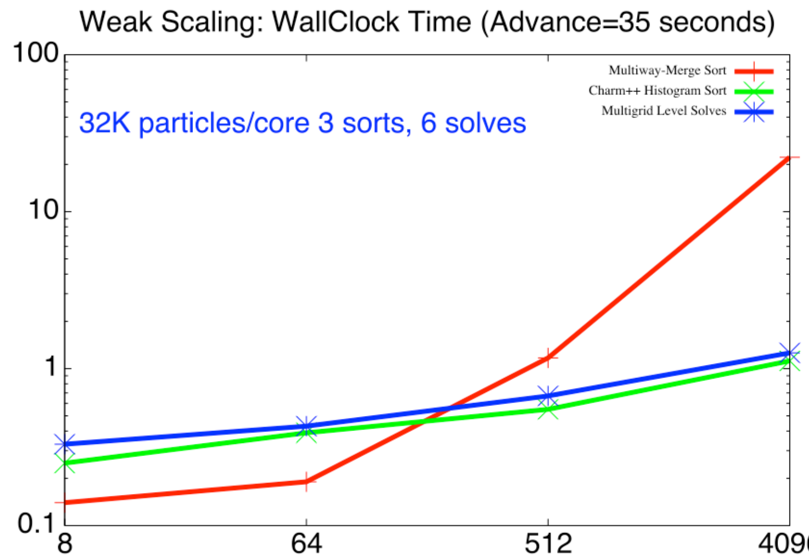
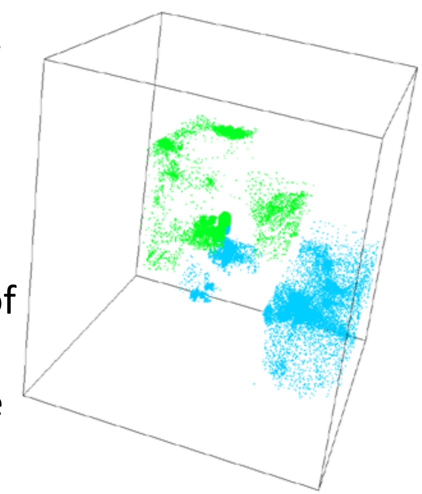
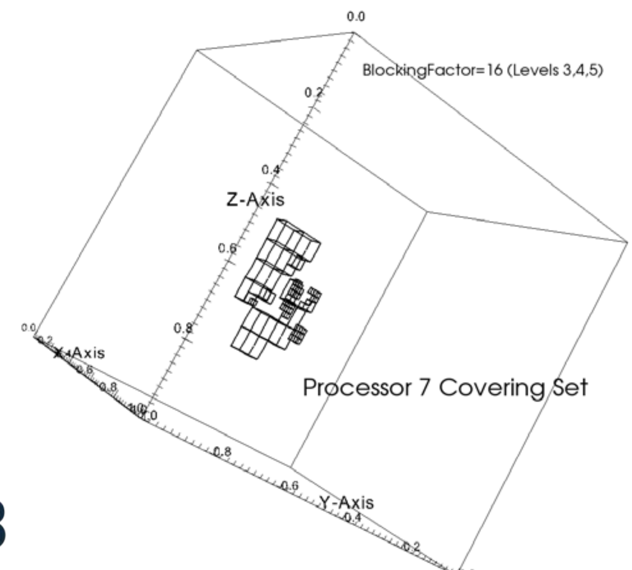
Advanced algorithms: two-grid schemes for PIC

- Using the same domain decomposition for the field solve grids and for the particle deposition results in load imbalance.
- For simulations for which the are a large number of particles per grid cell, we perform field solves and field-particle transfers with different grids.
- Particles handled with sorted space-filling curve, transfers to local "covering set" grids (distributed sorting can be hard!)
- The transfer between the two sets of grids is done efficiently, since the amount of field data is small relative to the particle data.







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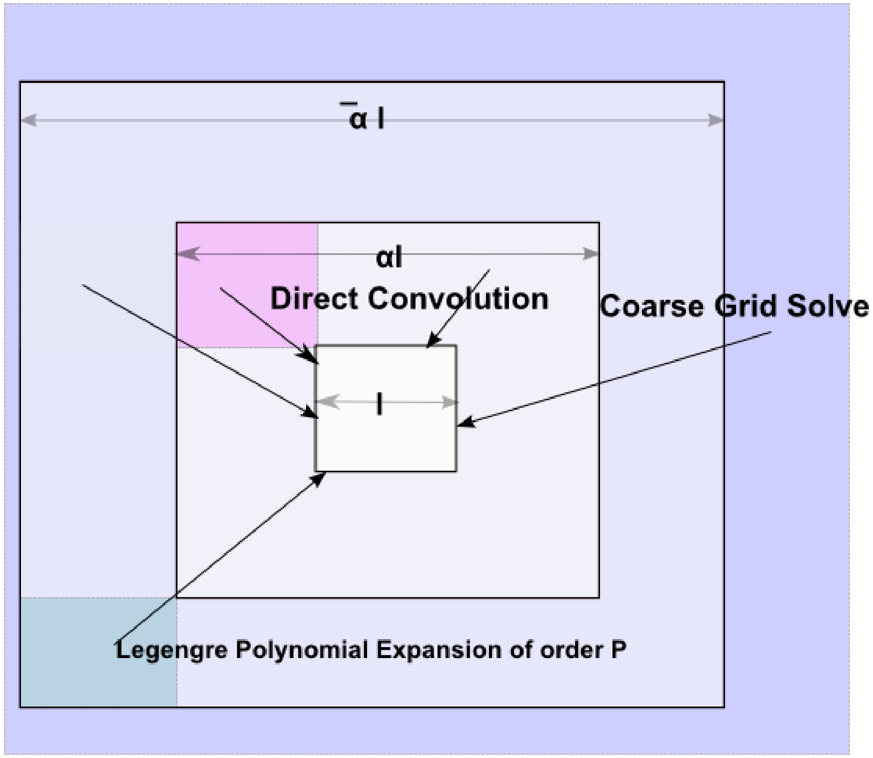
Advanced algorithms: method of local corrections

- Potential-theoretic domain - decomposition Poisson solver compatible with AMR grids
- One V-cycle solver
  - Downsweep: build RHS for coarser grids using discrete convolutions and Legendre polynomial expansions
    - exploits higher-order FD property of localization
    - Convolutions performed with small FFTs and Hockney 1970
  - Coarse solve
    - Either MLC again, or FFT
  - Upsweep
    - Solve for Φ_h on boundary of patch
    - Interpolation and summations
    - Local Discrete Sine Transform Solve



No iteration, accurate, no self-force problems, large number of flops per unit of communication (messages and DRAM).

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Conclusions

- PIC methods for accelerators now scale to the size of the biggest available machines
  - Multiple factors make this practical in production runs
- Working implementation of GPU/multicore-optimized algorithms
- Advanced algorithmic research underway