Argonne NATIONAL LABORATORY

... for a brighter future

Simulations of High-intensity Beams Using BG/P Supercomputer at ANL

J. Xu [1,2], B. Mustapha [1], V.N. Aseev [1]

and P.N. Ostroumov [1]

Physics Division [1]

Math. & Computer Science Division [2]

Argonne National Laboratory

9700 S. Cass Ave.

Argonne, IL 60439.

August 26 , 2008

U.S. Department of Energy

UChicago Argonne LLC

Office of Science U.S. DEPARTMENT OF ENERGY

Content

- **Status of Current Research**
  - LINACs: ATLAS, Fermi Lab. Proton Driver, SNS, ……
  - Supercomputers: Jazz, BG/P

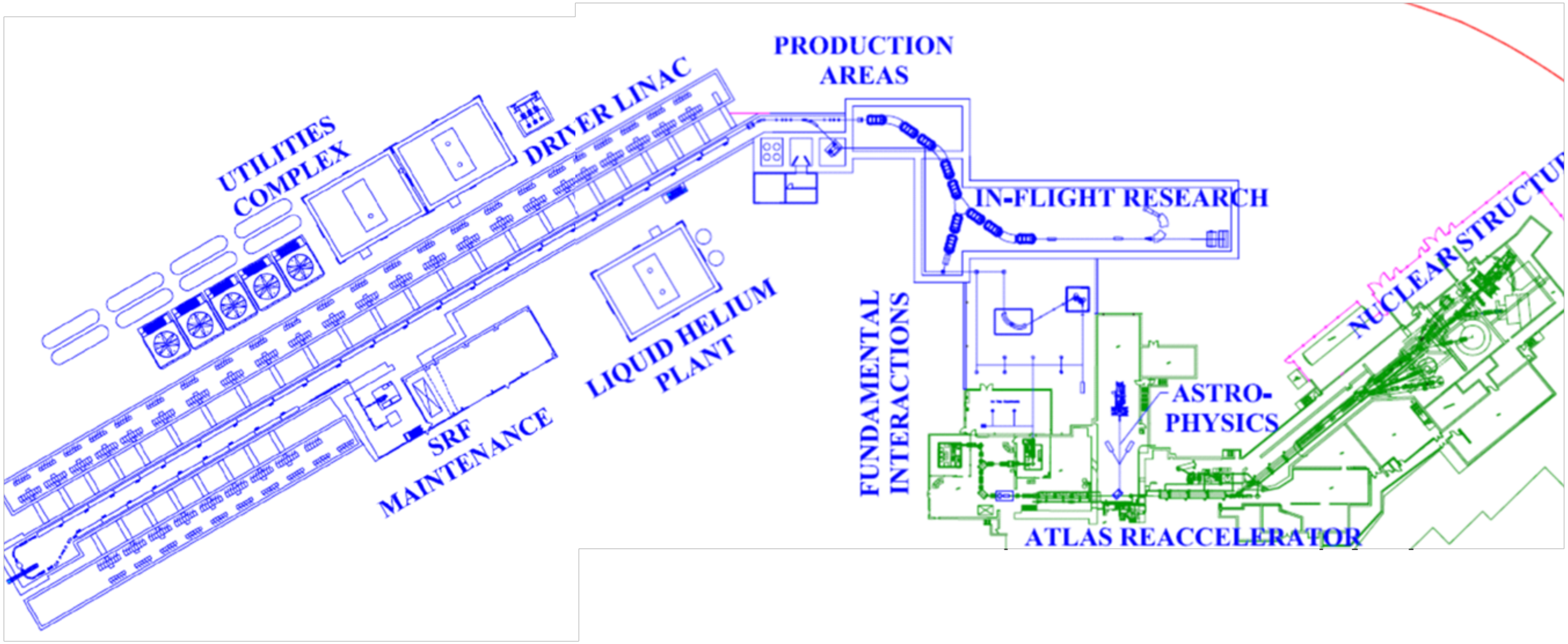
- **Numerical Method and Parallel Model**
  - TRACK: Design, Misalignment Error, Correction, ……
  - PTRACK: Parallel Model
  - Parallel Poisson solvers for Space Charge effect

- **Large Scale Beam Dynamics Simulations**
  - Challenges (I/O, Scaling,……)
  - Radio Frequency Quadrupole (RFQ)
  - Proton Driver at Fermi Lab. (PD)

- **Summary**

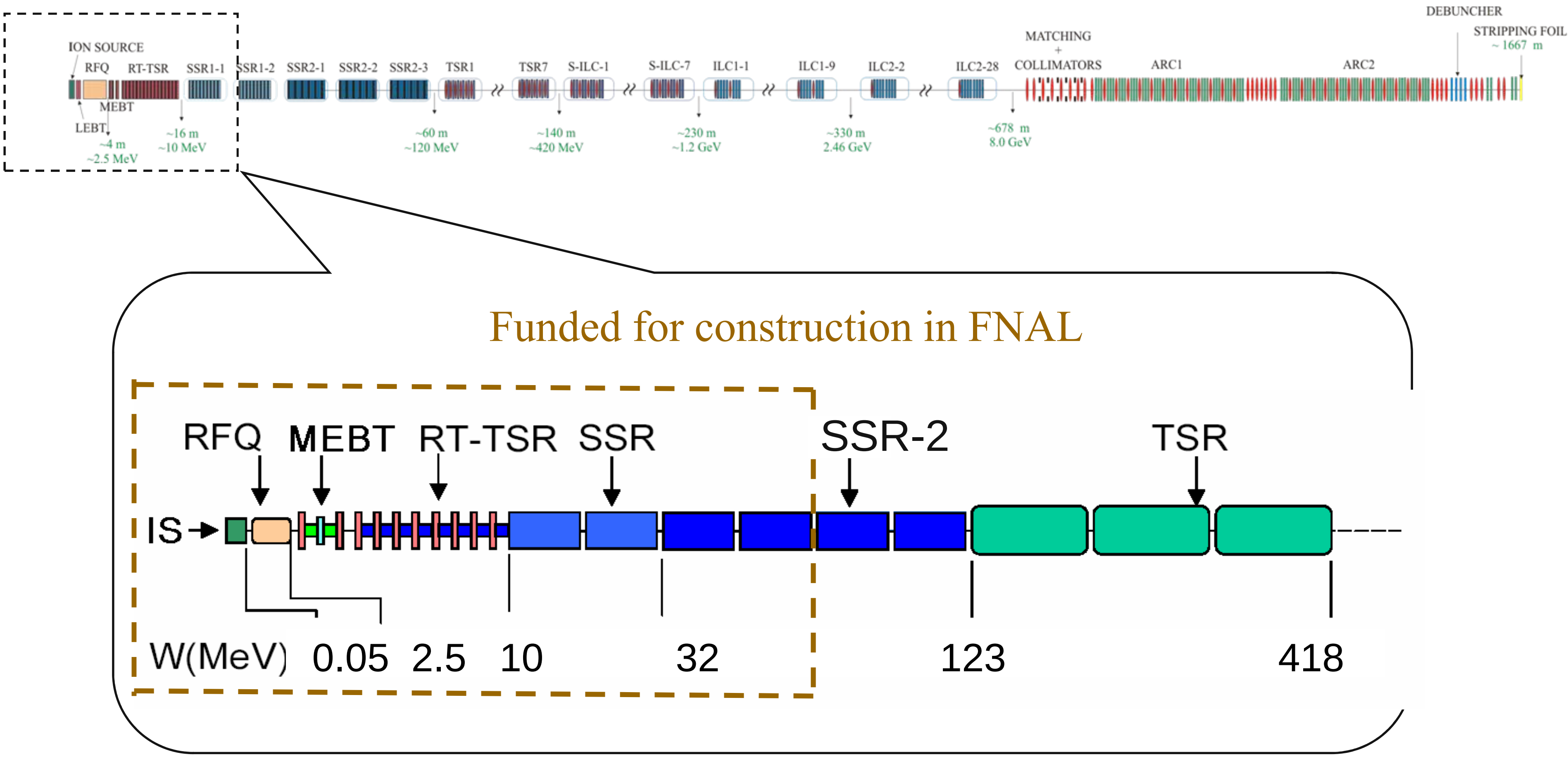
Facility for production of Rare Isotopes

- 800 MV SC Linac, beam lines, targets and post accelerator



Based on old 10MeV ATLAS Linac

8 GeV Fermi Lab. Proton Driver

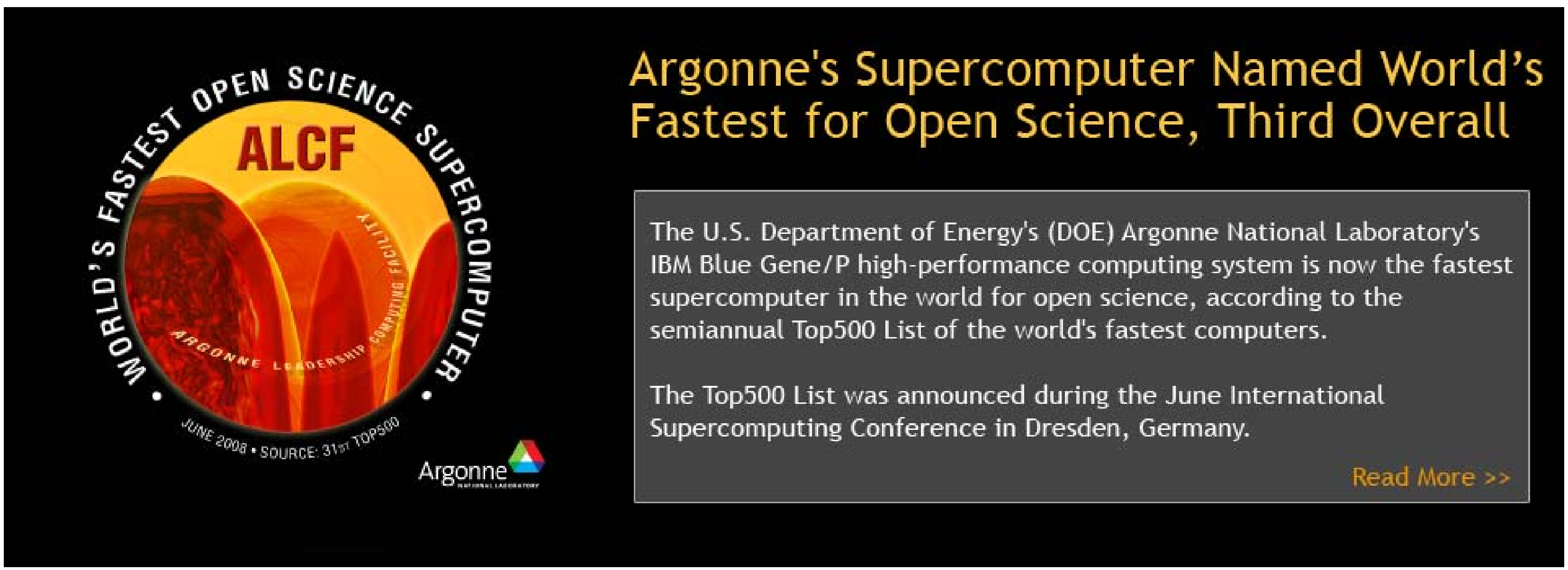


P.N. Ostroumov, New J. Phys. 8 (2006) 281. http://stacks.iop.org/1367-2630/8/281.

DOE Leadership Computing Facility (LCF) Strategy

DOE SC selected the ORNL, ANL and PNNL teams for LCF Strategy

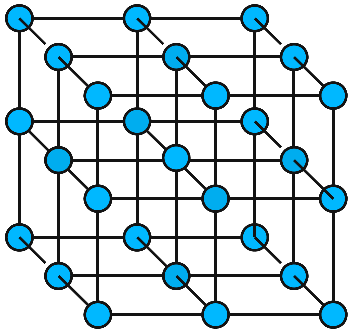
- ORNL will deploy a series of systems based on Cray's XT3/4 architectures @ 250TF/s in FY07 and 1000TF/s in FY08/09
- ANL will develop a series of systems based on IBM's Blue Gene @ 556TF/s in FY08/FY09 with IBM's Next Generation Blue Gene
- PNNL will contribute software technology



BG/P at ANL

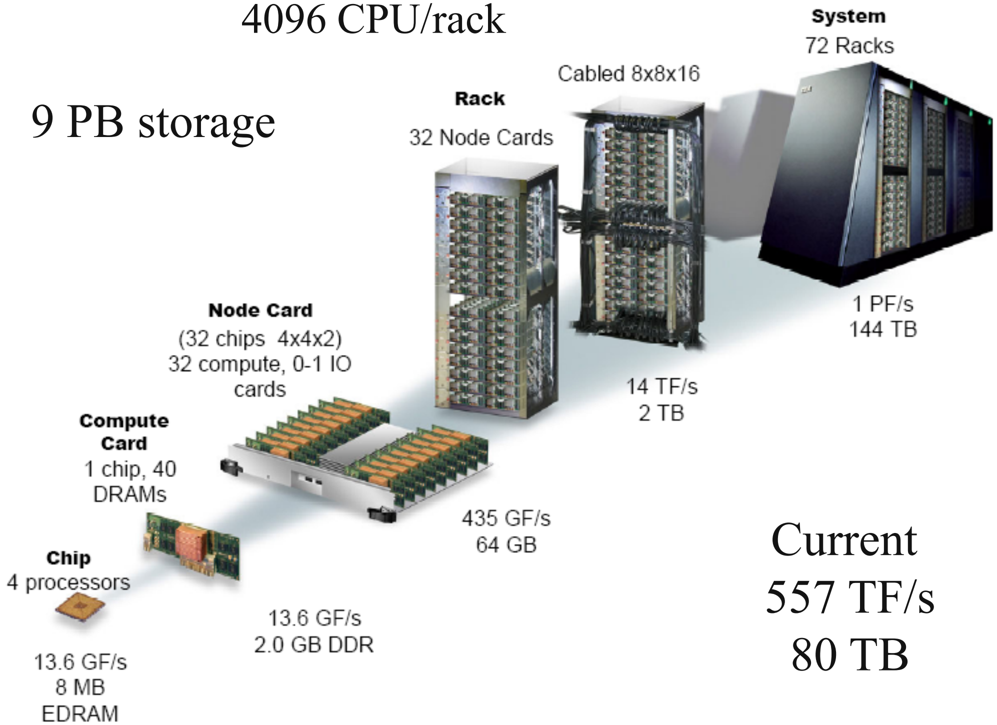
4096 CPU/rack

9 PB storage



3D torus network

10 GB/s between any node



Current

557 TF/s

80 TB

- **Surveyor (IBM Blue Gene/P):**
  - 1 rack, 1,024 quad-core nodes (4,096 processors)
  - 2 terabytes of memory.
  - Peak performance is 13.9 teraflops.
  - 512Mbs/processor

- **Intrepid (IBM Blue Gene/P)**
  - 40 racks, 40,960 quad-core nodes (163,840 processors)
  - 80 terabytes of memory.
  - Peak performance is 556 teraflops.
  - 512Mbs/processor

Numerical Method for Beam Dynamics Simulations

- PIC method has been used.
- Advantages: easy to implement, fast speed, small grid
- Disadvantages: Noise decreases as $1/\sqrt{N}$, hard to predict detailed beam structures, such as beam halo.

$$\frac{d\vec{\boldsymbol{x}}}{dt} = \frac{\vec{\boldsymbol{p}}}{\gamma m} = \vec{\boldsymbol{v}}$$

$$\frac{d\vec{\boldsymbol{v}}}{dt} = \vec{\boldsymbol{F}} = q\cdot(\vec{\boldsymbol{E}} + \vec{\boldsymbol{v}}\times\vec{\boldsymbol{B}})$$

$$= \boldsymbol{q}\cdot(\vec{\boldsymbol{E}}_{ext} + \vec{\boldsymbol{v}}\times\vec{\boldsymbol{B}}_{ext} - \nabla\phi)$$

Parallel Efficiency = Particle Tracking, 100% + Electromagnetic Fields, 0~100% (external EM and space charge)

Space Charge Effect:

$$\Delta\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} = -\frac{\rho}{\varepsilon_0}$$

$$= \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial\phi}{\partial r}) + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2} + \frac{\partial^2\phi}{\partial z^2}$$

$$\nabla\cdot\vec{E} = \frac{\rho}{\varepsilon_0}, \quad \nabla\cdot\vec{B} = 0$$

$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\nabla\times\vec{B} = \mu_0\vec{J} + \varepsilon_0\mu_0\frac{\partial\vec{E}}{\partial t}$$

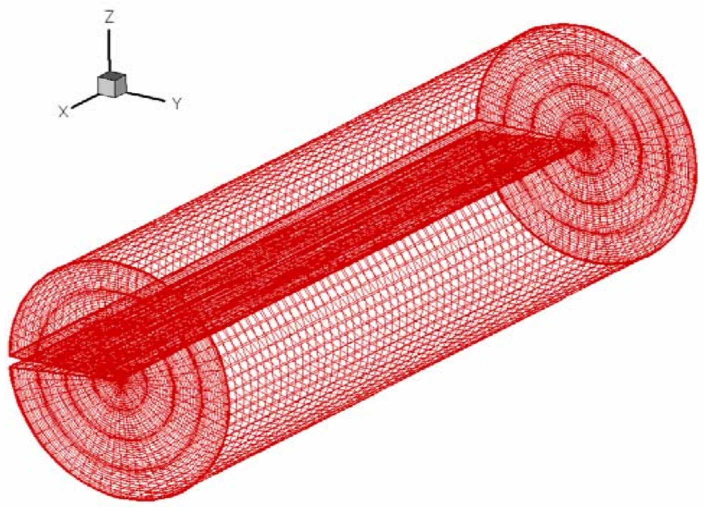
- Based on TRACK code which was developed at ANL since 1998
- TRACK is z-based LINAC tracking code
- TRACK focus on heavy ion beam with relativistic effect
- PTRACK was developed since 2005
- PTRACK includes nearly all accelerating devices in TRACK
- EM fields are provided by other software and each processor has a copy
- EM solvers are under development
- Particles are distributed evenly on all processors
- Include space charge effect by solving Poisson's equation
- Several parallel Poisson solvers have been developed
- In Cartesian coordinate system (FD, FE, Spectral, Wavelet, ……)
- In Cylinder coordinate system (Spectral and Spectral Element)
- 1D, 2D and 3D domain decompositions
- ……

PTRACK

Poisson's Equation in Cylinder Coordinate System

- ✓ Finite Difference Method
- ✓ Finite Element Method
- ✓ Fourier Spectral Method
- ✓ Spectral Element Method
- ➢ Fast Multi-pole Method
- ➢ Multi-grid Method
- ✓ Wavelet Method

……



$$\phi(x,y,z,t)=\sum_{m=-M/2}^{M/2-1}\sum_{n=-N/2}^{N/2-1}\sum_{0}^{P}\phi(m,p,n,t)e^{-i\alpha mx}e^{-i\beta nz}P_p(y)$$

$$P_p(y)=\begin{cases}(\frac{1-y}{2}) & p=0\\ (\frac{1-y}{2})(\frac{1+y}{2})P_{p-1}^{1,1}(y) & 0<p<P\\ (\frac{1+y}{2}) & p=P\end{cases}$$

$BC:$

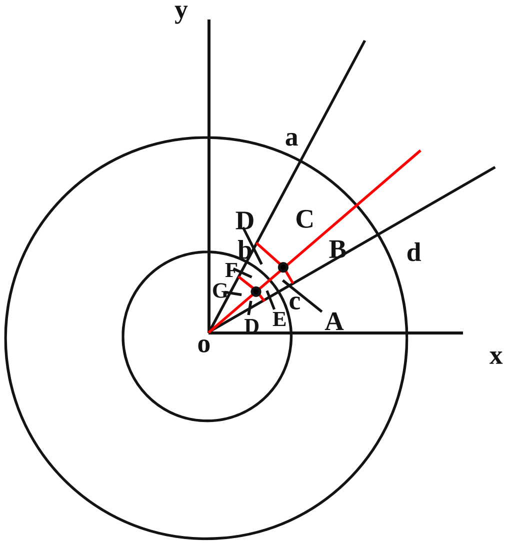
$$\phi(r=a,\theta,z)=0;\quad \phi(r=0,\theta,z)<\infty$$

$$\phi(r,\theta+2\pi,z)=\phi(r,\theta,z);$$

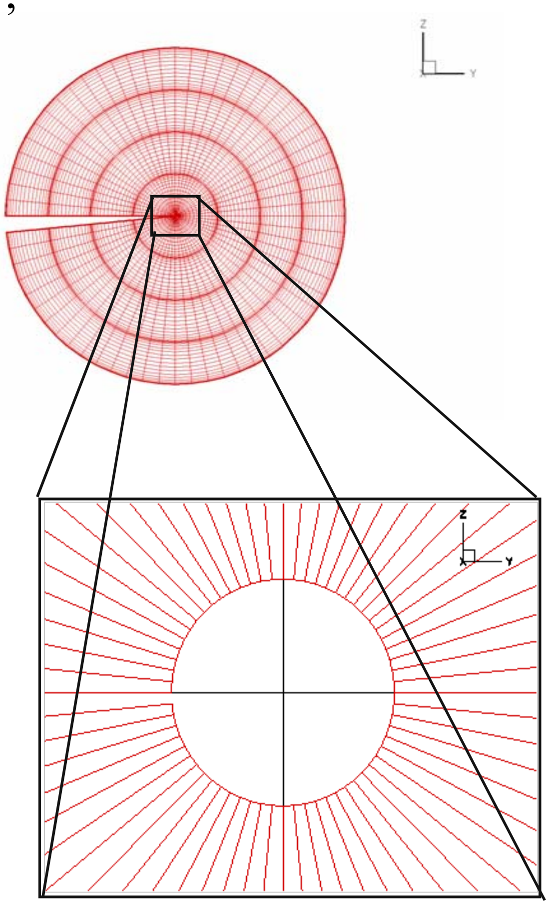
$$\phi(r,\theta,z)=\phi(r,\theta,z+L)$$

Parallel Poisson Solver in Cylindrical Coordinate System

$$q_a = \frac{A}{S}, q_b = \frac{B}{S}, q_c = \frac{C}{S}, q_d = \frac{D}{S},$$
$$S = A + B + C + D$$



$$q_o = \frac{E+F}{S}, q_b = \frac{D}{S}, q_c = \frac{G}{S},$$
$$S = D + E + F + G$$



$$A \cdot \tilde{\phi} = \hat{f}, \quad A = K + M + N$$

$$K_{pq} = \int_0^1 r \frac{\partial \phi_p(y)}{\partial r} \frac{\partial \phi_q(y)}{\partial r} dr$$

$$M_{pq} = m^2 \int_0^1 \frac{1}{r} \phi_p(y) \phi_q(y) dr$$

$$N_{pq} = n^2 \int_0^1 r \phi_p(y) \phi_q(y) dr$$

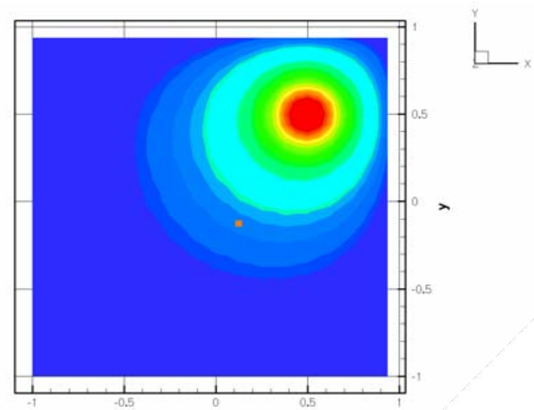
Linear system

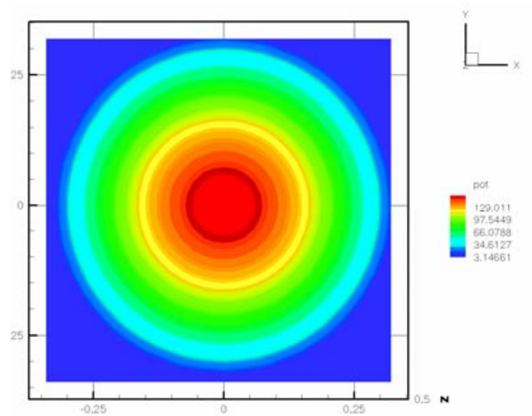
Gauss-Lobatto-Radau

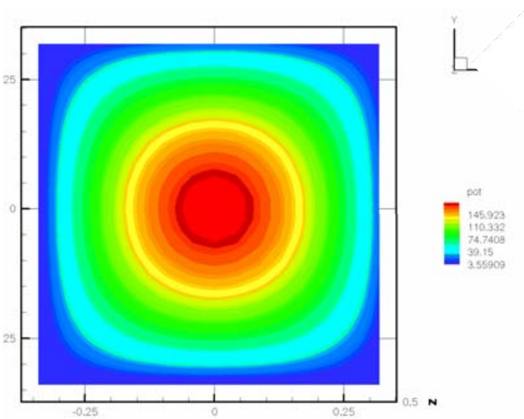
$$(-1.0, 1.0]$$

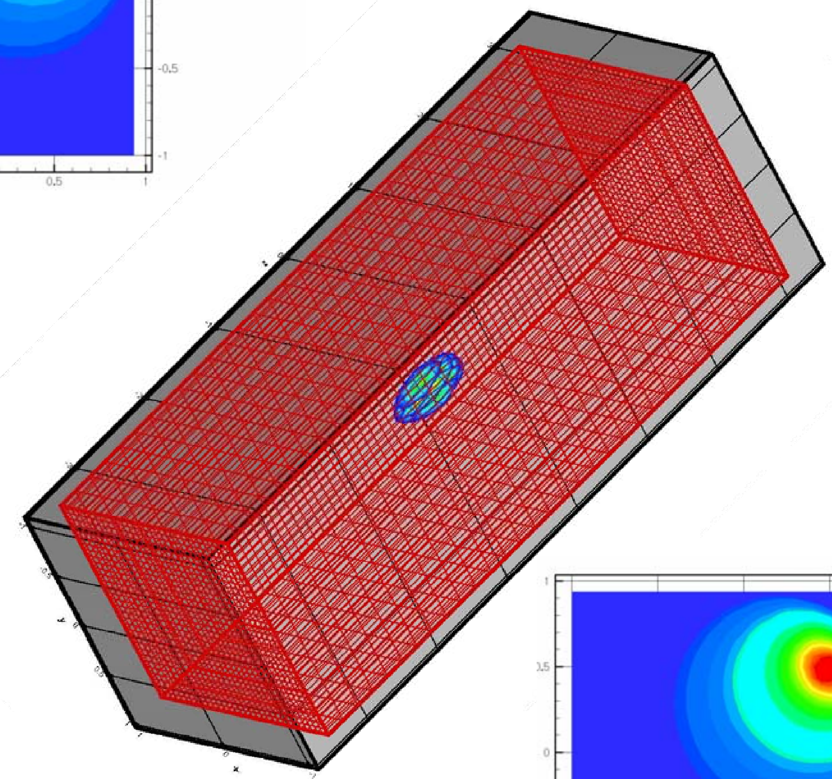
• J. Xu and P.N. Ostroumov, "*Parallel 3D Poisson Solver for Space Charge Calculation in Cylinder Coordinate System*", Computer Physics Communications, 178 (2008) 290-300.

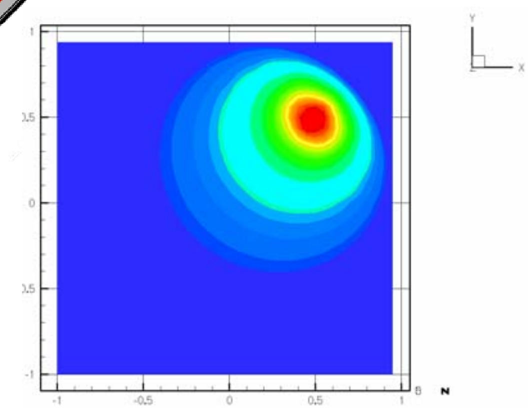
Potential Comparison on Cartesian and Cylindrical Coordinate Systems





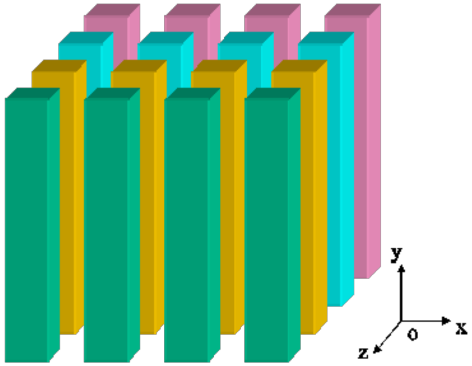




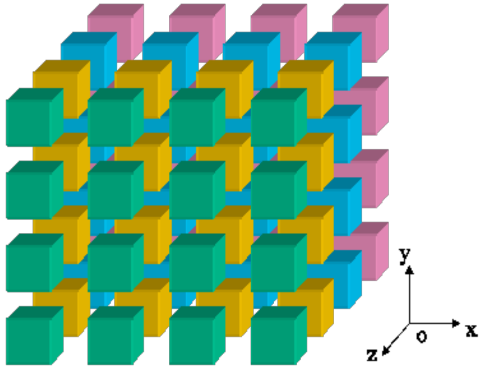


Parallel Models for Poisson's Equation

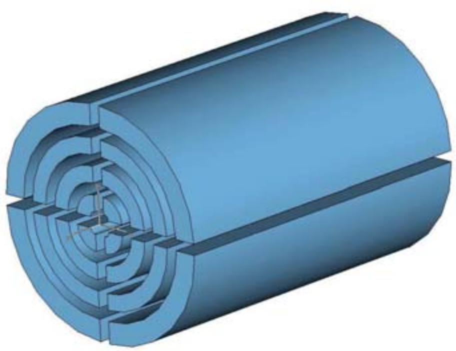
Model A

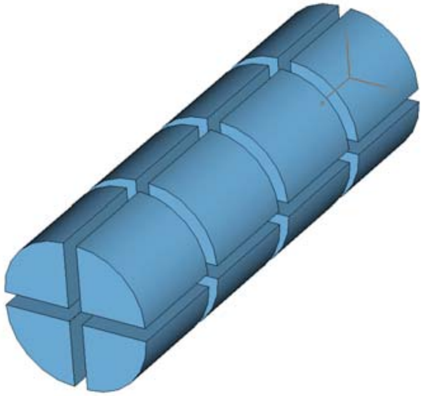


Model B



Model C

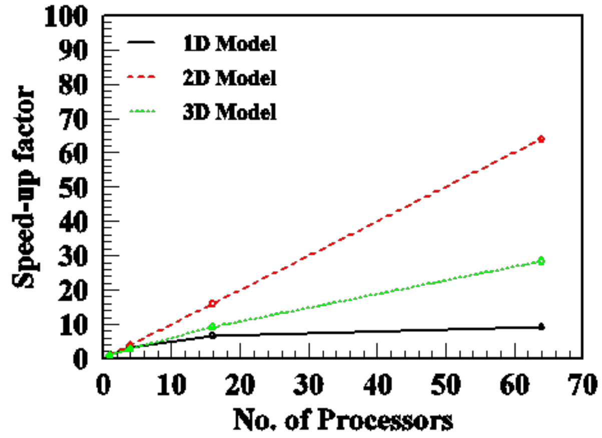


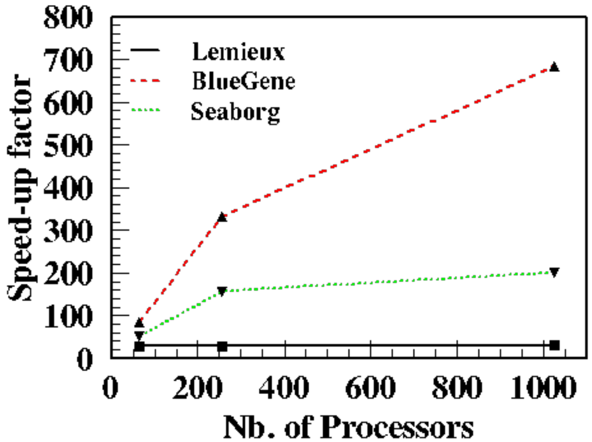


- ✓ MPI + Fortran
- ✓ FFTW3 for FFT, Fast Sine Transform (Real even DFT)
- ✓ BLAS, LAPACK libraries

Benchmarks and Simulation Results

$$u(x,y,z,t)=\sum_{m=-M/2}^{M/2-1}\sum_{p=-P/2}^{P/2-1}\sum_{n=-N/2}^{N/2-1}\hat{u}(m,p,n,t)e^{-i\alpha mx}e^{-i\beta py}e^{-i\gamma nz}$$





Mesh $128\times128\times256$

Three Parallel Models

$$\Delta U=\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}+\frac{\partial^2 U}{\partial z^2}=-\frac{\rho}{\varepsilon_0}$$

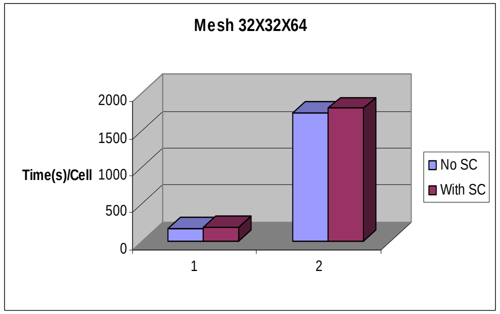
Particle# $\dfrac{\text{SC}}{\text{Tracking}}$

100K------10%

1M ------3.7%

100M ------0.037%

$32\times32\times64$

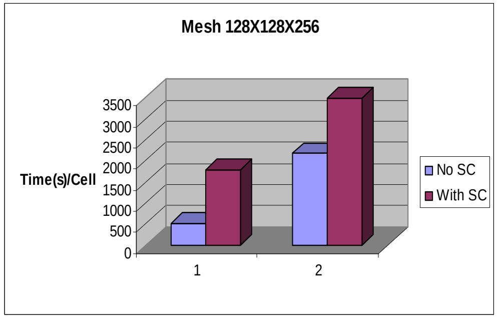


100K------246%

1M ------59.7%

100M ------0.597%

$128\times128\times256$



Why Large Scale Computing?

- Provide more advanced support for accelerator science, reduce cost for accelerator design, commission and operation.
- Can overcome shortcoming of PIC method by simulating real number of particles in beam bunch
- Speed up simulations and shorten simulation time
- More accurate and detailed simulations, important to investigate more complicated phenomena, such as halo, beam losses, etc.
- Study more misalignment errors by simulating larger number of particles and seeds to improve the LINAC optimizations
- Investigate more challenging problems which can lead to new scientific discoveries!

Challenges

- **Parallel I/O**
  - For better performance, each directory has maximum one thousand files
- **Memory**
  - Each processor has only 512 MB memory, load balance
- **Post-processing**
  - Transferring 160GB to hard drive takes 74 hours! (600KB/s)
  - Takes 4.5 hours with 10MB/s network bandwidth!
  - Suppose one file I/O takes one second, 32K files takes 9.1 hours for I/O!
- **Storage**
  - 865,000,000 particles generate 160GB data
  - 10,000,000 particles with 100 seeds generate 175GB data
- **Parallel Poisson solver**
  - Maximum # of processors (1 grid point/processor)
  - For 32K cores, $256\times128\times128$ SC mesh in 2D and $32\times32\times32$ in 3D parallel Poisson solver (128 times smaller!)
  - Scaling problem

PTRACK's Weak and Strong Scaling

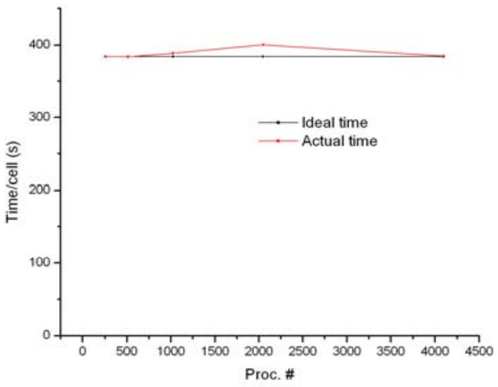
Table. Weak scaling of PTRACK with 64^3 mesh for space charge

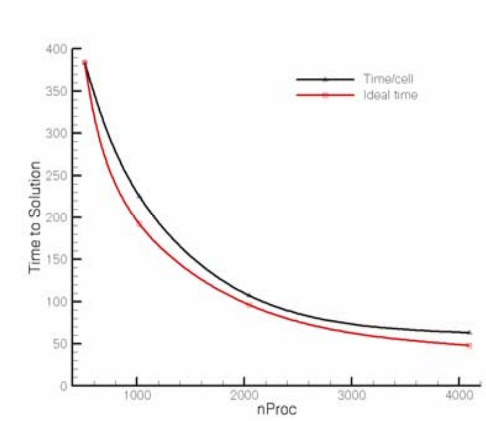
CPU	Time/cell (s)	Particle #	Parallel Efficiency
256	384	55M	100%
512	384	110M	100%
1024	388.7	220M	98.8%
2048	400.6	440M	95.8%
4096	385	880M	99%

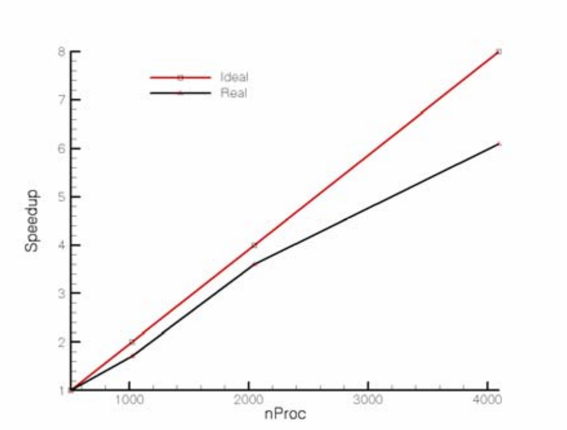
Table. Strong scaling of PTRACK with 64^3 mesh for space charge, 110M particles

CPU	Time/cell (s)	Ideal Time (s)	Parallel Efficiency
512	384	384	100%
1024	225	192	85.3%
2048	107	96	89.7%
4096	63	48	76.1%

Parallel Efficiency







Particle#	1M	10M	100M	865M
CPU#	1024= 16*16*4	4096= 16*16*16	4096= 16*16*16	32768= 32*32*32
Particle/CPU	1k	2.56k	25.6k	26.4k
SC Grid	$32\times32\times32$	$32\times32\times32$	$32\times32\times32$	$32\times32\times32$
I/O time(s)	14	110	36	135
Tot Time(h)	0.63	1.06	6.3	? 4.8

Large Scale Beam Dynamics Simulations using PTRACK

- ATLAS
  - ✓ 100 millions particles full simulation
- Radio Frequency Quadrupole (RFQ)
  - ✓ 100 millions particles full simulation
  - ✓ 865 millions particles part simulation
  - ✓ 865 millions particles full simulation
- Fermi Lab. Proton Driver Linac (PD)
  - ✓ 100 millions particles simulation
  - ✓ 100 seeds with 10 millions particles each
  - ✓ 865 millions particles simulation

$$\boxed{100 \times 10^7 = 10^9}$$

One billion particle statistics!

- ❖ Spallaton Neutron Source (SNS)
- ❖ Facility for Rare Isotopic Beam (FRIB)

☆ 100K particles takes 14 hours with 1 CPU
While with 16 CPU, takes 1 hour;
And with 64 CPU, takes **20 minutes!**

☆ 1,000,000 particles on BG takes 5.5 days!
Now with 64 CPU, takes about 2.2 hours!
And with 256 CPUs, it only takes **38 minutes!**

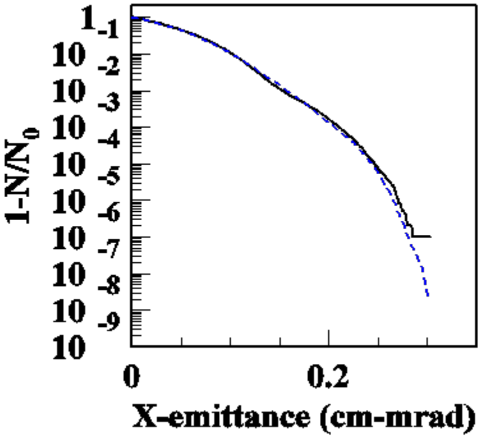
☆ Now we can simulate **865M** particles through RFQ with 32,768 CPU in 5 hours.

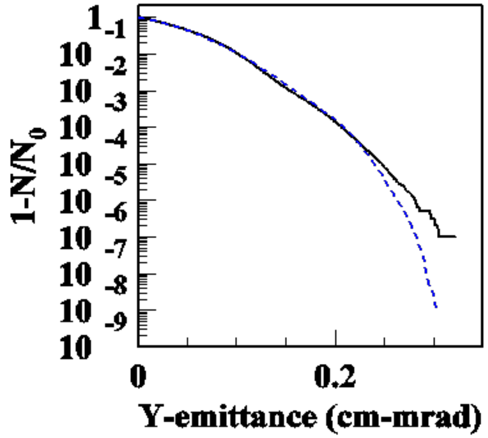
☆ Using BG/P with 65,536 CPU, it is possible to simulate ~ **Billions** of particles.

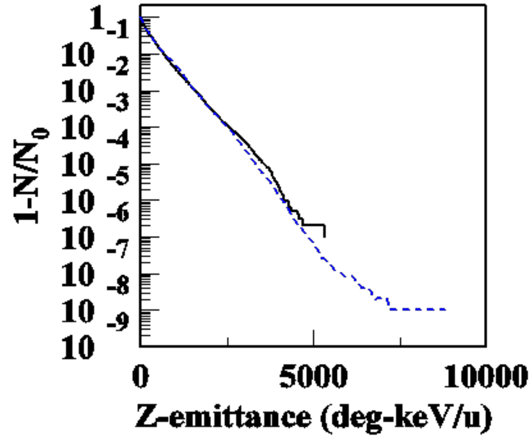
☆ 10^{11} particles still is a challenge

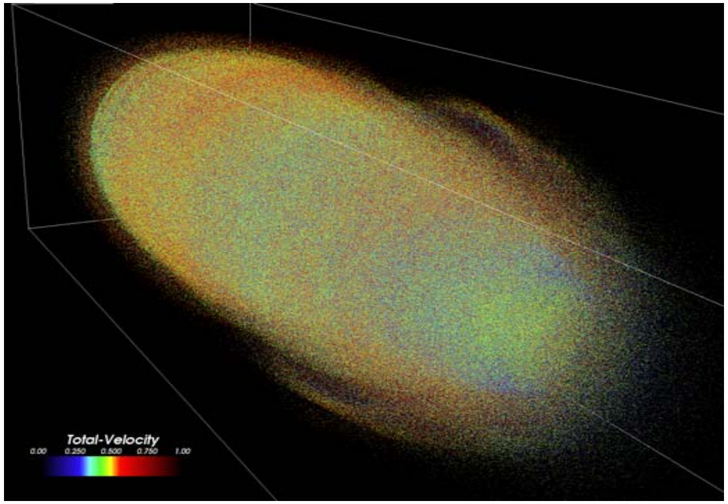
Simulation Results: RFQ

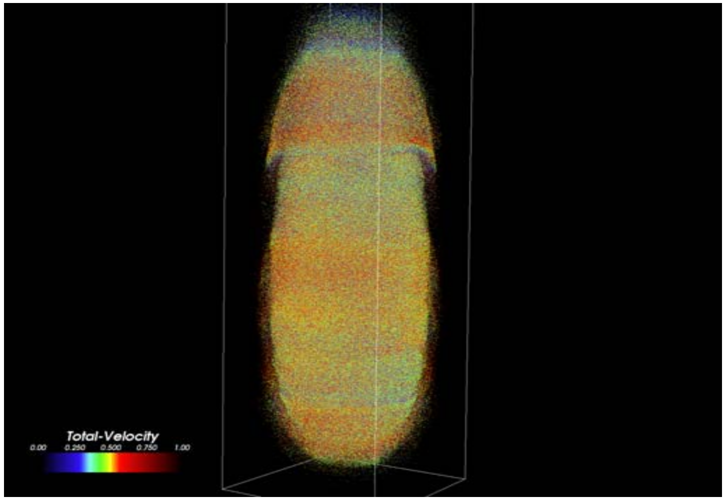
1M vs. 100M particles







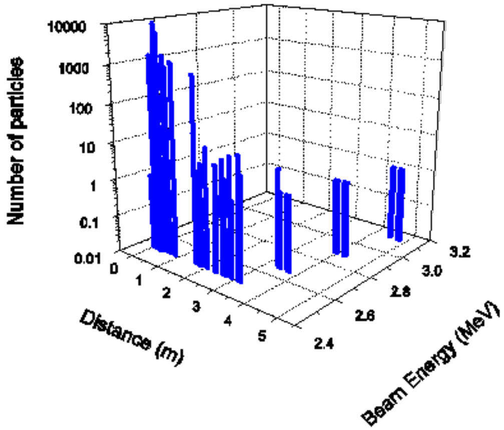




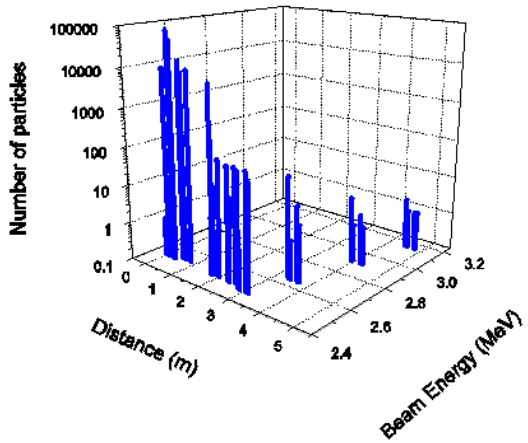
100,000,000 particles

Courtesy of JB Gallagher

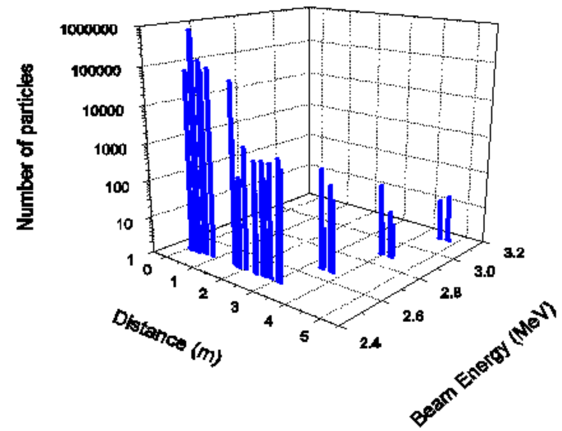
Comparison



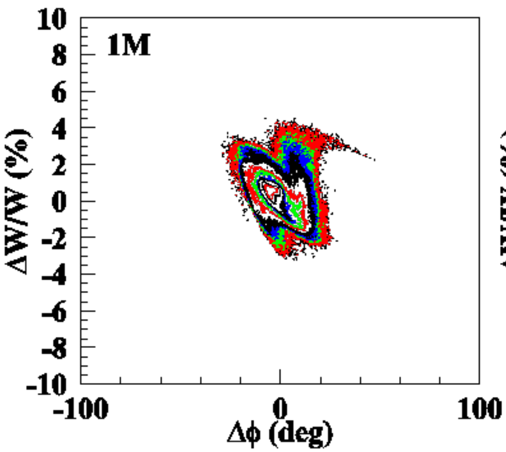
1M

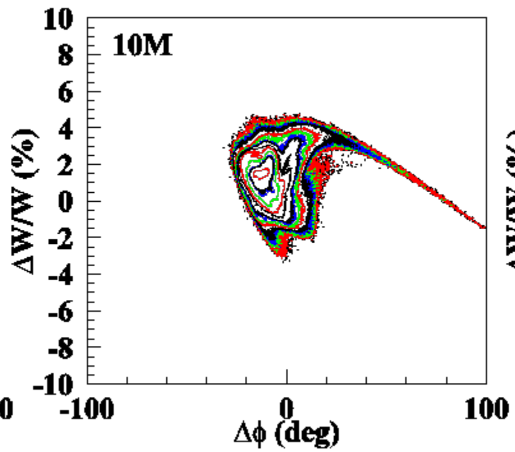


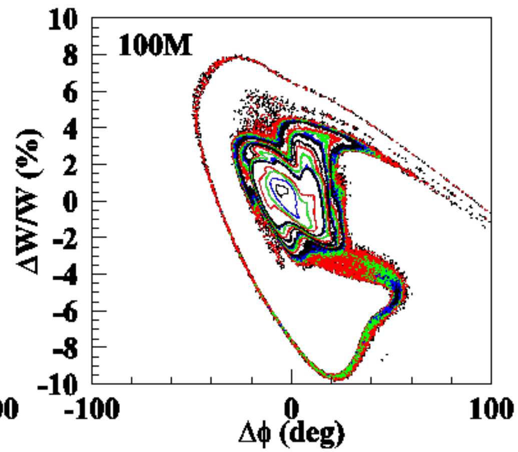
10M



100M

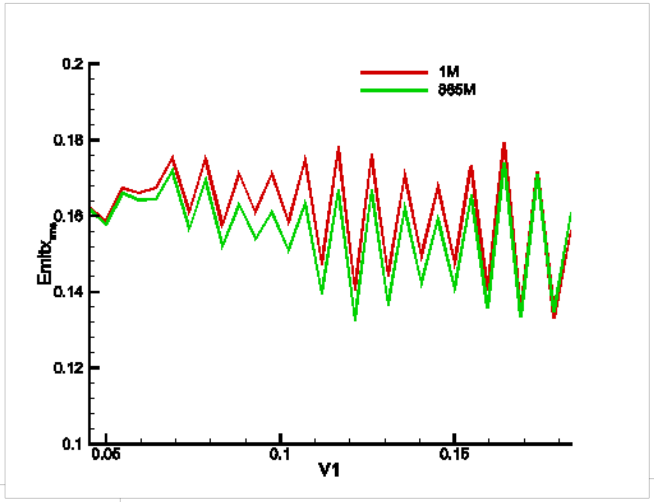


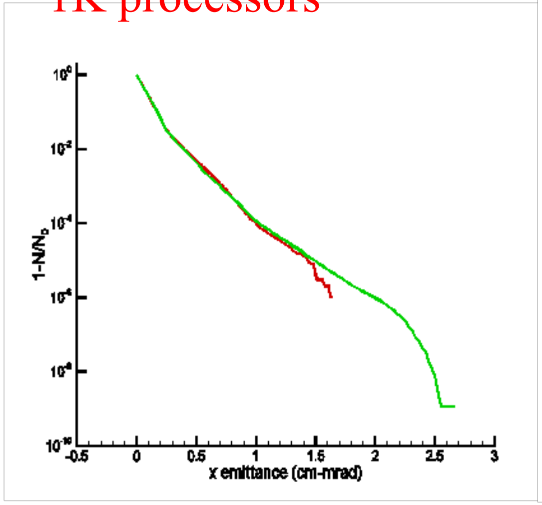




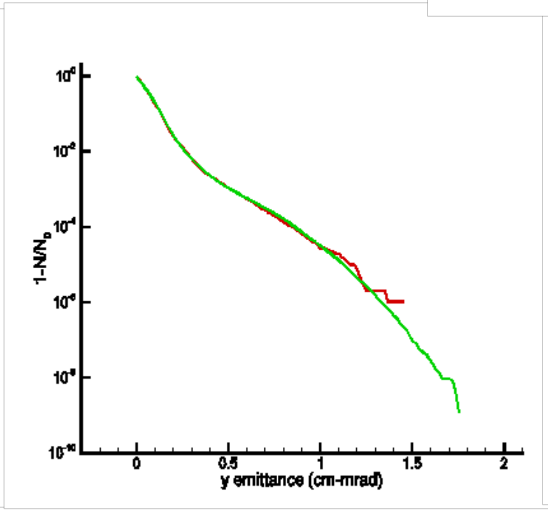
One-to-one Simulation Results in RFQ:

- Real bunch in Proton Driver has about 865,000,000 particles
- 269 cells RFQ (Only simulate the first 30 cells now)
- Input RFQ energy 50keV
- Output RFQ energy 2.5 MeV
- 2 hours using 32,768 processors
- 150 GB/time step
- 2 minutes I/O
- Post-processing takes about 20 minutes on 1K processors

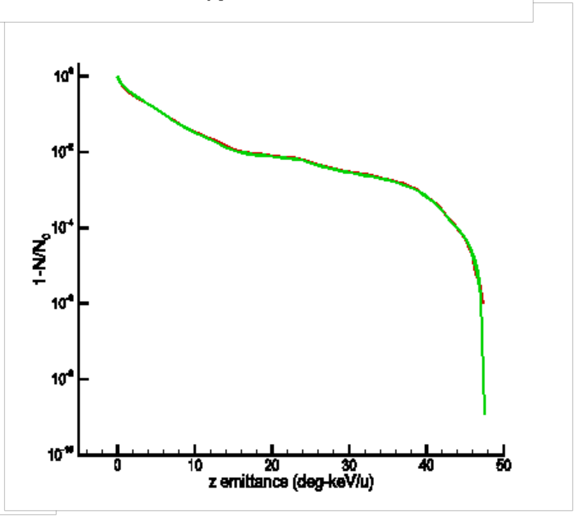




x



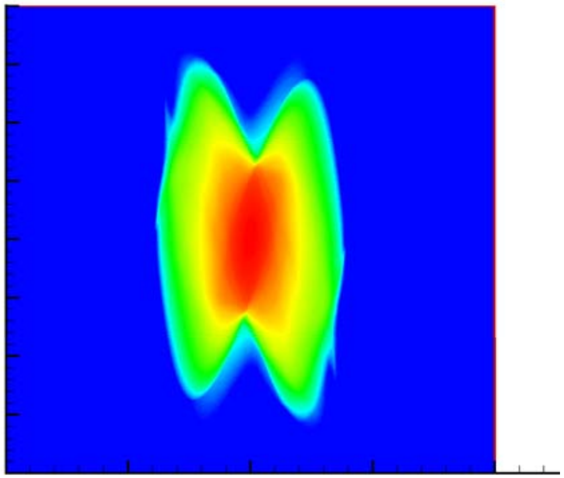
y

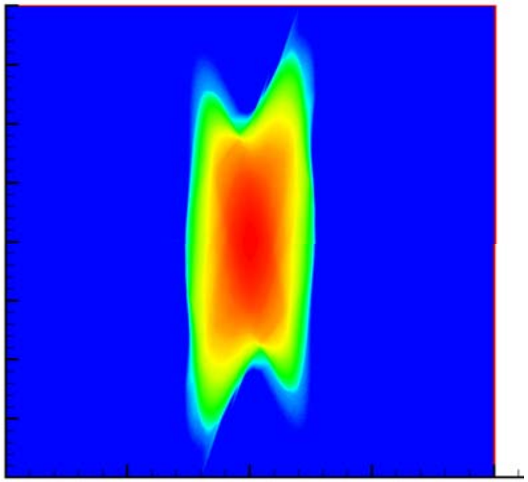


z

Phase Contours

(x, x')

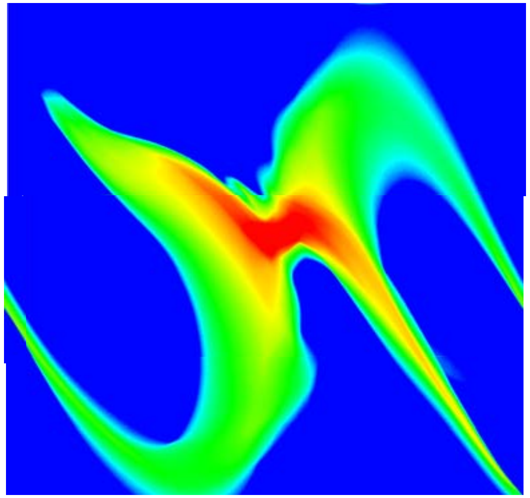


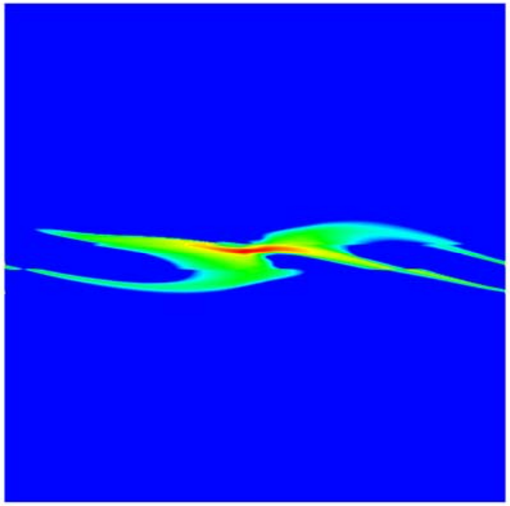


(y, y')

865M particles
after 30
RFQ cells

(t, dw)



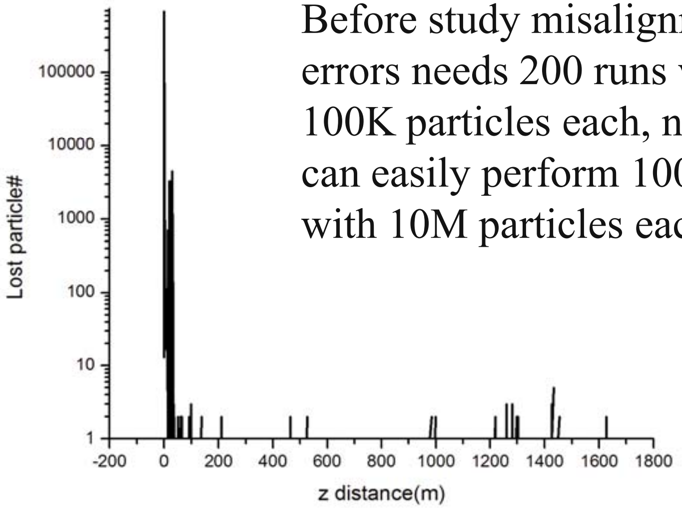


W=50.86keV
Freq=325MHz

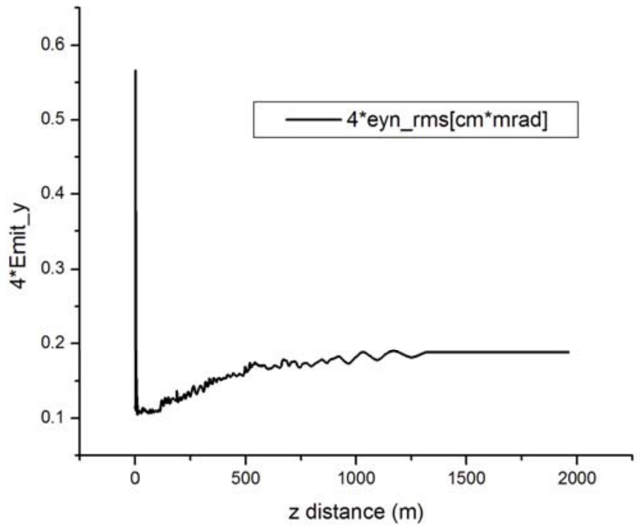
(phase, dw/w)

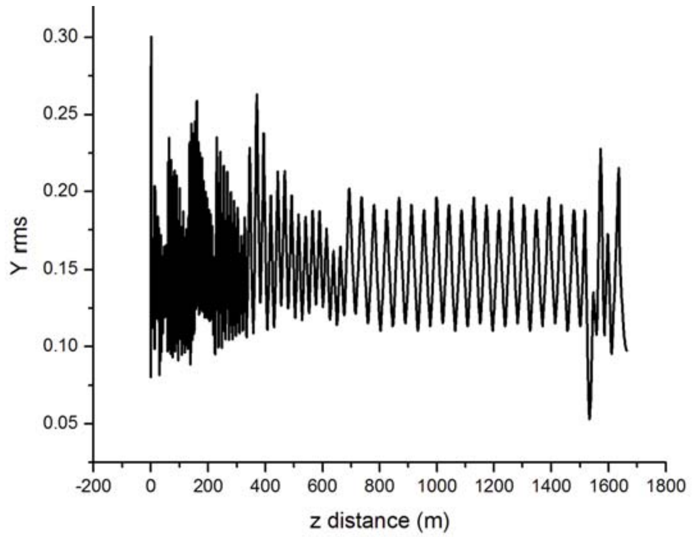
Proton Driver Simulation Results

- 100M H^- particles
- Three Stripping:
  Residual Gas,
  Magnetic field,
  Black Body Radiation)
- 2.5MeV to 8 GeV
- 1.6 km long
- Takes 6.5 hours on 4K processors



Before study misalignment errors needs 200 runs with 100K particles each, now we can easily perform 100 runs with 10M particles each.





Summary

- PTRACK has been successfully upgraded to run on BG/P system
- Several parallel Poisson solvers have been developed and incorporated into PTARCK
- Using small grid for space charge, good scaling has been demonstrated on BG/P system up to 32K processors
- Real one-to-one beam dynamics simulation for RFQ can be done on BG/P using 32K processors
- In the future, parallel post-processing has to be completed
- End-to-end simulations can be performed for RFQ, Fermi Lab. Proton Driver, SNS LINAC, etc.
- PTRACK has and will greatly improve high intense beam dynamics simulations for LINAC.