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A parallel approach for Monte Carlo-based photon propagation simulation

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Introduction

- The aim of this paper is to emphasize the advantages of using the high-performance computing in the field of high-energy physics simulations based on Monte Carlo technique.

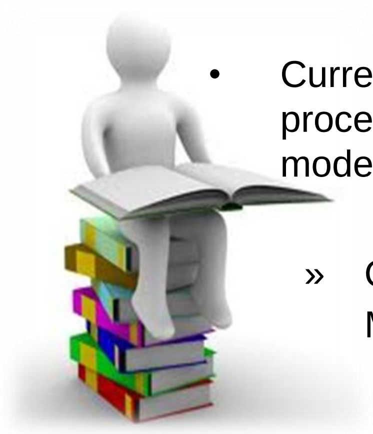
- In particular, the problem took under the study is the photon propagation through a multilayered medium, which is in many ways the simplest problem of radiation transport.

- The most important part of this project is to develop a CBEA-based Monte Carlo algorithm optimized to be executed on IBM Roadrunner cluster from our HPC Laboratory.

- The Monte Carlo method offers a great accuracy of solution, but has a big disadvantage: the method is high time-consuming. For this reason, the majority of research in this area has focused on the development the techniques based on high performance computing.

- Currently, we are working on a parallel Monte Carlo algorithm optimized for Cell/B.E processors which is based on a well known Monte Carlo model – MCML (Monte Carlo modeling of light transport in multi-layered tissues).

  » Our work is concentrated in developing techniques of parallelization and optimization of Monte Carlo simulation algorithms specific to the CBEA-based clusters.



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HPC resources @ USV
USV Roadrunner cluster

IBM RoadRunner cluster BladeCenter QS22/LS22 PowerXCell8i 3.2 GHz
(the same architecture as number 1 in the Top 500 of the Supercomputers in June 2009)

- 48 blade servers QS22 with 96 PowerXCell8i processors 3.2 GHz
- 8 blade servers LS22 with AMD Opteron processors
- TB storage capacity
- the hybrid architecture's computing power in double precision (proved by Linpack) is 6.53 TFlops

High Performance Computing Laboratory of the
Faculty of Electrical Engineering and Computer Science
„Ştefan cel Mare" University of Suceava

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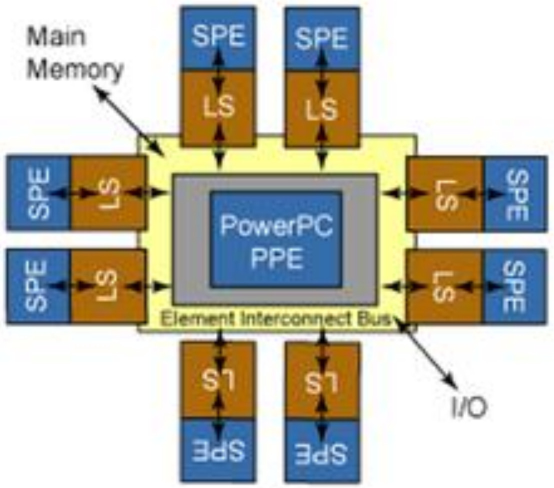
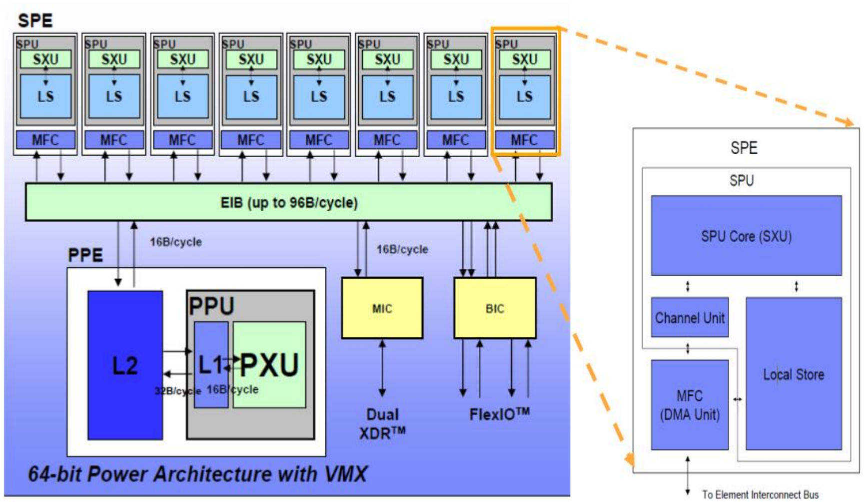
CBEA: Cell Broadband Engine Architecture



- The **PPE (The POWER Processing Element)** is the main processor of the Cell BE, and is responsible for running the operating system and coordinating the SPEs.
- The key design goals of the PPE are to maximize the performance/power ratio as well as the performance/area ratio.
- The PPU is a dual-issue, in-order processor with dual-thread support.



- The **SPE** is a modular design consisting of a **Synergistic Processing Unit (SPU)** and a Memory Flow Controller (MFC).
- An SPU is a compute engine with SIMD support and 256KB of dedicated local storage.
- An SPU is a dual-issue, in-order machine with a large 128-entry, 128-bit register file used for both floating-point and integer operations.

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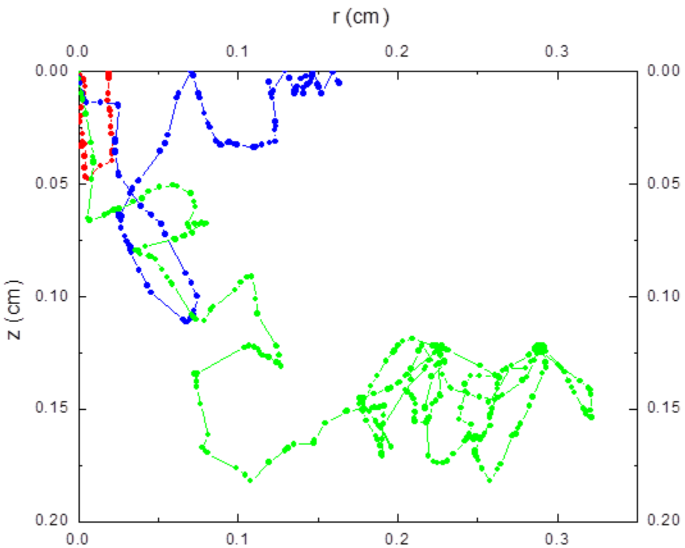
Monte Carlo Simulation for Radiation Propagation Problem



What is it?

Method used to solve mathematical and physical problems by the simulation of random variables.

How is it works in simulation of high-energy particles transport?

» simulate how a particle evolves step by step in radiation propagation
» each step in particles propagation and each interaction occurred are computed using random numbers.

MC codes

EGSnrc / BEAMnrc | PENELOPE | MCNPX | GEANT4 | MCML

Challenges to overcome

Reduce computation time (maintain accurac

HPC Solution
PARALLEL MC

HPC solution :: Cell/B.E.-MCML

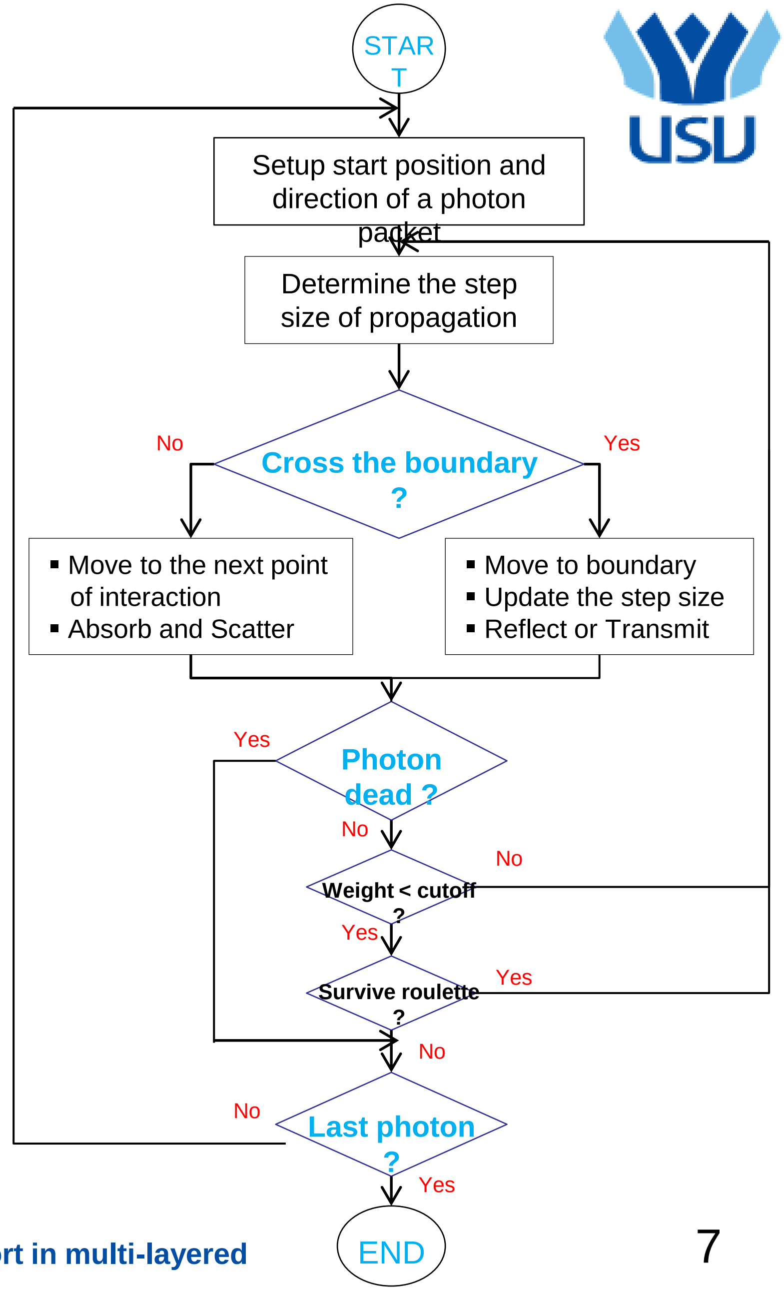
We started from *MCML code which is a well known Monte Carlo model of light transport in multilayered tissues.

MCML is a steady-state Monte Carlo simulation program for multi-layered turbid media with an infinitely narrow photon beam as the light source.

Each layer has its own optical properties of absorption, scattering, anisotropy, and refractive index. The simulation is 3D, but the results are stored in an r-z array in cylindrical coordinates denoting radial and depth positions.

Outputs include the radial position and angular dependence of local reflectance and transmittance, and the internal distribution of energy deposition within the multilayered medium.

The program can be easily modified.

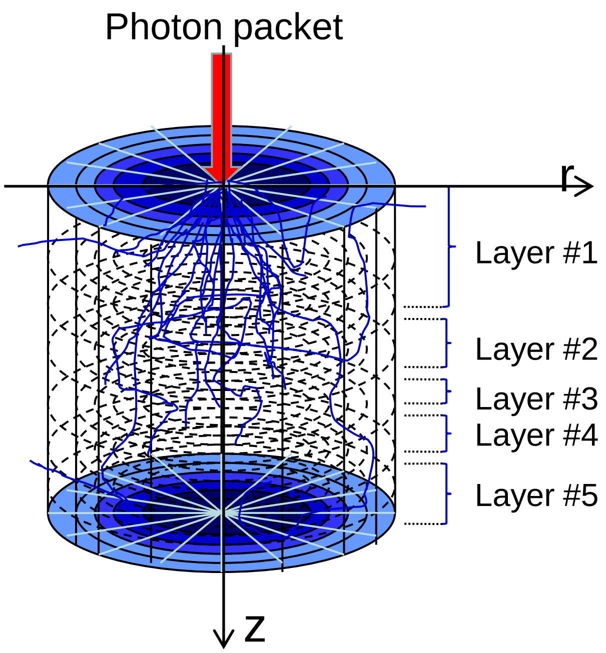


* Wang, L.-H., et al. (1995). "MCML - Monte Carlo modeling of photon transport in multi-layered tissues."

Input parameters of MCML code :: optical parameters and geometry description

Sample.mci

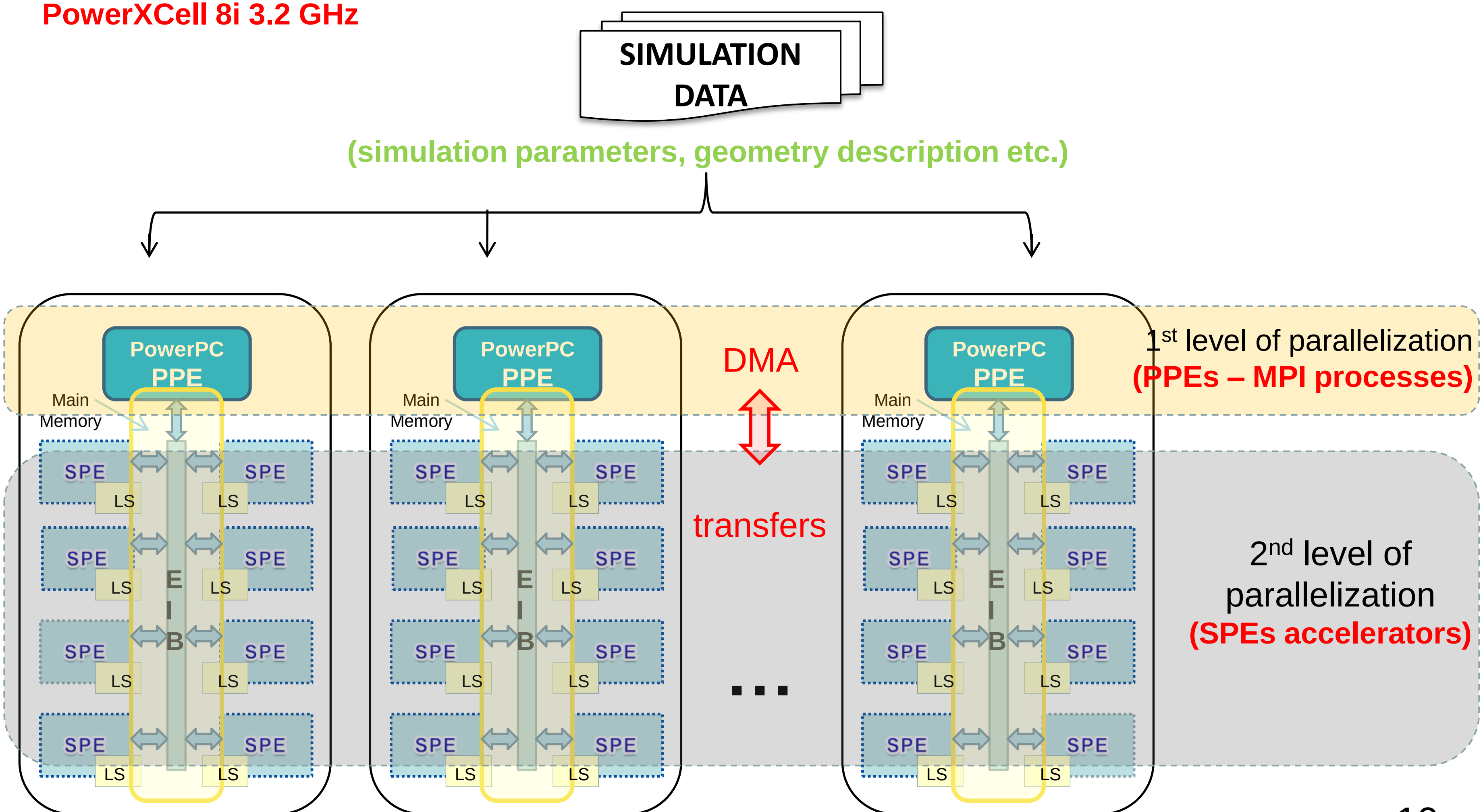
```
####
# Template of input files for Monte Carlo simulation (mcml).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
# Meglinsky et al. "Modelling the sampling volume for skin
# blood oxygenation measurements"
####

1.0                         # file version
1                           # number of runs

### Specify data for run 1
test1.mco A                 # output filename, ASCII/Binary
1200                        # No. of photons
0.002 0.01                  # dz, dr
500 200 30                  # No. of dz, dr & da.

7                           # No. of layers
# n mua mus g d             # One line for each layer
1.0                         # n for medium above.
1.53 0.2 1000 0.9 0.002     # layer 1: stratum corneum
1.34 0.15 400 0.85 0.008    # layer 2: living epidermis
1.4 0.7 300 0.8 0.01        # layer 3: papillary dermis
1.39 1 350 0.9 0.008        # layer 4: upper blood net dermis
1.4 0.7 200 0.76 0.162      # layer 5: dermis
1.39 1 350 0.95 0.02        # layer 6: deep blood net dermis
1.44 0.3 150 0.8 0.59       # layer 7: subcutaneous fat
1.0                         # n for medium below.
```



- are highly parallelizable because:
  - a lot of particles have to be processed
  - a lot of random numbers have to be processed
  - particles interact with the material only, not with each other
  - the geometry, material and fields which the particle is traversing are static, i.e. they do not change with the particle interactions

Cell/B.E.-MCML :: implementation considerations

IBM Cluster BladeCenter QS22/LS22
PowerXCell 8i 3.2 GHz

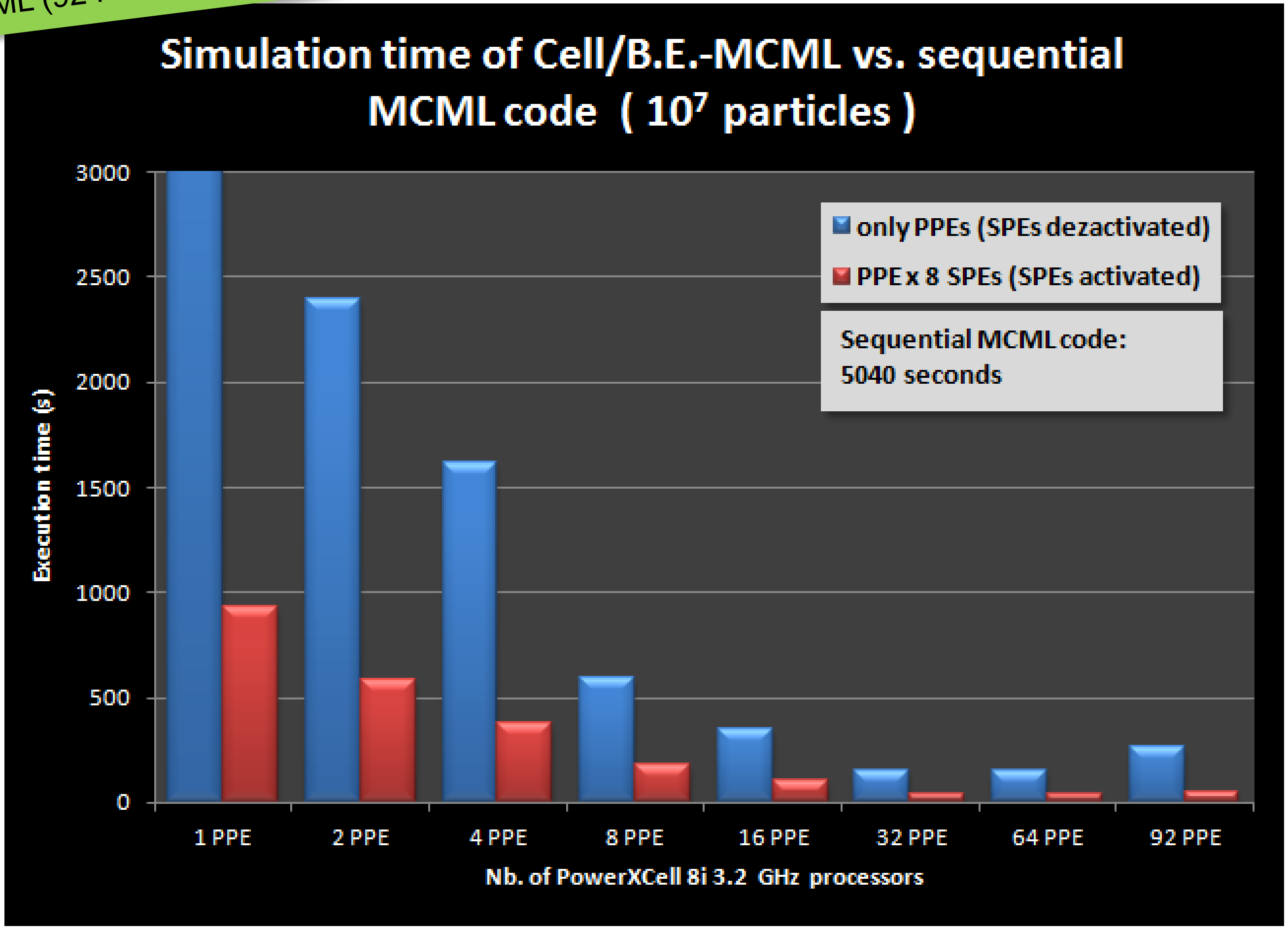


Cell/B.E.-MCML :: results

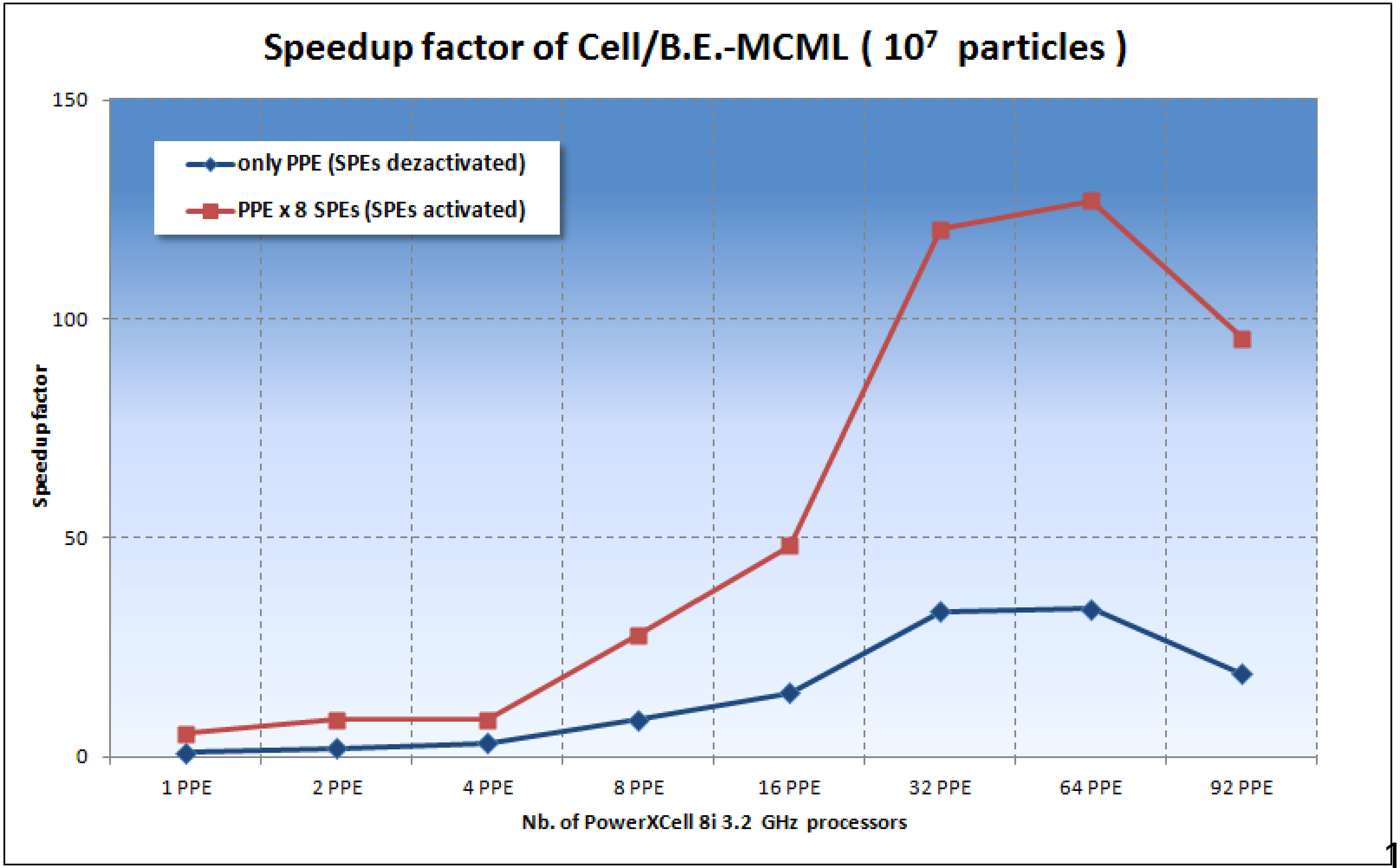
Simulation time of 10^7 photons

» CPU-MCML (IBM PowerXCell8i 3.2GHz): **1.4 hours**

» Cell/B.E.-MCML (92 PPE x 8 SPE accelerators cores): **less than 1 minute**



Cell/B.E.-MCML :: results



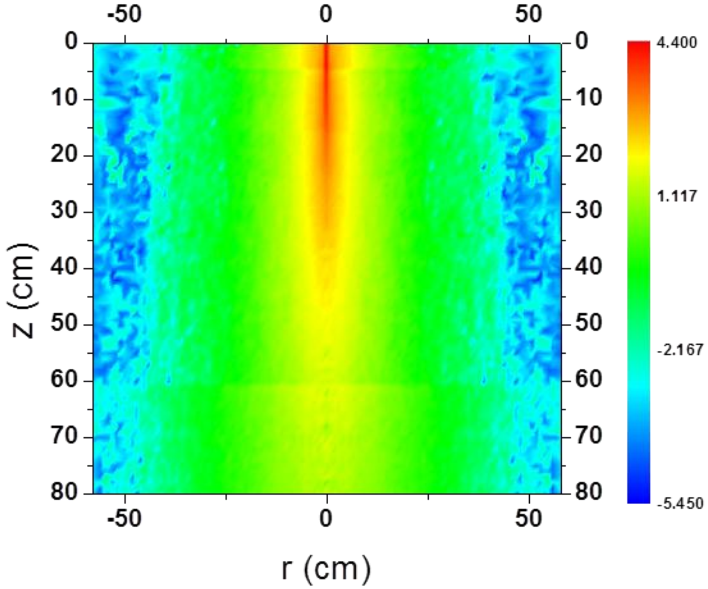
Cell/B.E.-MCML :: validation of simulation

Tests were performed on medium described below:

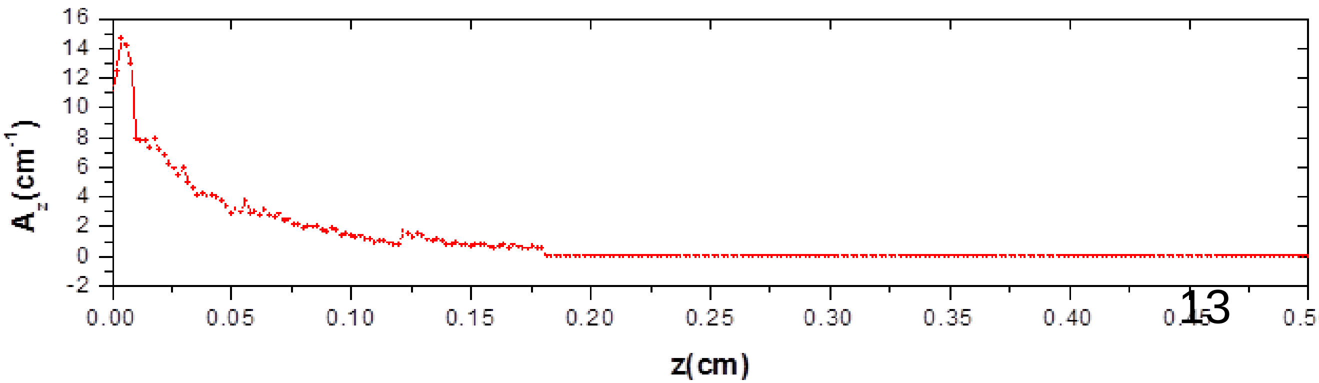
0.002 0.01 # dz, dr
500 200 30 # No. of dz, dr & da.
7 layers

# n	mua	mus	g	d
1.53	0.2	1000	0.9	0.002
1.34	0.15	400	0.85	0.008
1.4	0.7	300	0.8	0.01
1.39	1	350	0.9	0.008
1.4	0.7	200	0.76	0.162
1.39	1	350	0.95	0.02
1.44	0.3	150	0.8	0.59

Absorbtion (r,z) [W/cm³]



1D Absorbtion (z) [cm⁻¹]



Conclusions

- The Monte Carlo method offers a great accuracy of solution, but has a big disadvantage: the method is high time-consuming. For this reason, the majority of research in this area has focused on the development the techniques based on high performance computing.
- Considering the preliminary results obtained on Cell/B.E. processors, we can point out some features of the Monte Carlo method applied to radiation transport:
  - » the Monte Carlo method becomes more advantageous to the analytical method as the number of interactions increases interest and complicated geometry problem.
  - » the precision with which quantities of interest are estimated by Monte Carlo method (dispersion or variation thereof) depends on the number of particles observed: for example, for a small number of particles there will be typical of their trajectories.
  - » computing time increases with the number of tracked trajectories.
- The first attempts of developing a parallel Monte Carlo simulation for photon propagation showed us encouraging results, the compute power of PowerXCell8i processor demonstrating again its potential, and the advantages of IBM Roadrunner architecture.

ACKNOWLEDGMENT

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Thank you for your attention !