A top to bottom framework approach to vectorization

A. Gheata for the GeantV team
CHEP 2018
9-13 July 2018, Sofia, Bulgaria
"A view on performance"

by Homer Simpson

"You need to go faster for Run 3 !!!"

"Manufacturers made a better model for you! It's called AVX-512"

"SIMD is about many doing the same thing at once..."

"For efficiency, some synchronization is also needed"

"But... I've reached the theoretical limit for the stroke rate!..."

"Tried it with my best paddle, doesn't go faster ..."

"I understand now..."

"Can I use my old whistle?"
Beyond loop vectorization

Scalar data

Vector data “basketizing”

Online

Simulation, tracking, analysis

A top to bottom vectorization approach, CHEP’18
Complex workflows in vector approach


Buffer more inputs

Buffer outputs to next stages

Stage

Stage

Stage

buffer → Stage → selector

Top level functional algorithms become dispatching “stages”

Branching -> selective streaming

Vectorize lower-level algorithms and feed more particles at once

A top to bottom vectorization approach, CHEP’18
Both scalar/vector flow are supported

A top to bottom vectorization approach, CHEP’18
The bottom view: core components

Abstraction layer: [https://github.com/root-project/veccore](https://github.com/root-project/veccore)
Common math, RNG, …: [https://github.com/root-project/vecmath](https://github.com/root-project/vecmath)

- Vectorization of low-level algorithms using VecCore
  - See ”Vectorization of ROOT Mathematical Libraries” [talk](#) by L. Moneta for VecCore details
  - Geometry (M.Gheata [talk](#)), physics (M. Bandieramonte [talk](#)), propagation in field
  - Vectorizing on multi-particle inputs, but also on internal loops when possible

![Trapezoid benchmark on Xeon Phi](image)

- Haswell Core i7, AVX, Vc backend
The top view: simulation stages

- After having validated a realistic application against Geant4, we need to understand the performance
  - Detailed profiling of the simulation stages
- Many stages containing already vectorized code
  - Field propagation giving expected speed-up in the full flow
  - Not yet the case for geometry and post step action physics stage
- Thorough benchmarking against equivalent Geant4 application ongoing
  - Baseline for future optimizations
Profiling a realistic application

- Understanding hotspots
- Understanding basketization overheads
- Working on reducing scalar bottlenecks

A top to bottom vectorization approach, CHEP’18
Benchmarking configurations

- Magnetic field ON/OFF, propagator type
  - Understand behavior of different component implementations
- Basketizing ON/OFF (Physics, field, geometry in future)
  - Understand vectorization efficiency
- Basketize but perform scalar loops
  - Understand framework bottlenecks for basketizing
- MT simulation
  - Understand scalability, memory footprint
- Corresponding profiles generated
- Putting in place systematic performance monitoring

A top to bottom vectorization approach, CHEP’18
Current generic performance benchmark

CMS geometry, 100 GeV e⁻ isotropic gun

- Generic benchmark with standard EM processes for e⁺, e⁻, γ, field ON/OFF
- Full geometry imported from GDML, including production cuts
- Scoring:
  - mean energy deposit
  - mean charged and neutral step lengths
  - mean number of steps
  - mean number of secondary particles

Speedup FullCMS
Xeon® E5-2630@2.40GHz
gcc 7.3 AVX2, Vc backend

Best realistic case speedup vs. Geant4: ~60%

A top to bottom vectorization approach, CHEP'18
Ongoing work

• After understanding the main bottlenecks, now working on:
  • More vectorization work and connection of existing vectorized code
    • Multiple scattering and photoelectric model
  • Reducing basketization overheads
    • Light version (no track exchange among threads)
  • Geometry optimizations
    • Specialized volume navigators (reducing scalar bottlenecks + de-virtualizing + caching)
  • Physics optimizations + new features
    • Tuning usage of sampling methods depending on model and energy/material
    • Use of floating point instead of double case by case
  • Work on pRNG to support reproducibility in MT + basketized mode

• Aiming for a factor of ~2x for the full CMS benchmark for the beta tag end 2018 compared to Geant4
  • Out of which 25-40% from basket vectorization
Outlook

- Top to bottom vectorization on input data opens new optimization opportunities in simulation but not only
  - New algorithms become vectorizable
  - Pipeline workflows are perfect candidates, but more complex workflows can also benefit
  - Basketizing data comes with benefits (better caching, vectorization), but also overheads (data copying, larger memory footprint)

- Benefits of basketized approach become visible in GeantV
  - Not as large as initially expected due to the large complexity of simulation code
  - A detailed profiling analysis and optimizations ongoing

- Beta release of GeantV by the end of 2018
  - Demonstrator for realistic simulation of EM showers in the context of LHC
GeantV collaborators

- **BARC (India)**: S. Behera, A. Bhattacharyya, H. Kumawat, R. Sehgal
- **CIC-IPN (Mexico)**: J. Martínez Castro, A. Miranda Aguilar
- **FNAL (USA)**: D. Elvira, G. Lima, K. Genser, P. Canal, SY Jung, K Pedro
- **Students 2017-2018**: R. Schmitz, V. Drogan, S. Sharan, E. Orlova, Ananya, D. Savin

Thank you!