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Porting a Legacy Global Lagrangian PIC Code on Many-Core and GPU-Accelerated Architectures

PASC Conference, Basel

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EUROfusion

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Outline

Motivation

- Problem:
  - Development timescale of legacy code ORB5 [Tran, 1999, Jolliet, 2009] exceeds HPC architecture evolution timescale

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- Adopted strategy:
  - Disentangle numerical kernels and physical modules ⇒ modularization
  - More and more cores per compute node ⇒ trade multitasking for multithreading
  - Keep portability ⇒ directive-based approach (OpenMP and OpenACC)
  - Develop testbed code with fondamental kernels (PASC project)

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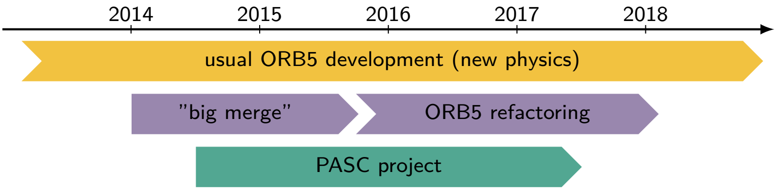
Recipe

- Timeline:



- Tools:
  - Profiler
    Score-P
    Scalable performance measurement infrastructure for parallel codes
  - Continuous integration tool
    Jenkins

ORB5, a multi-physics code...

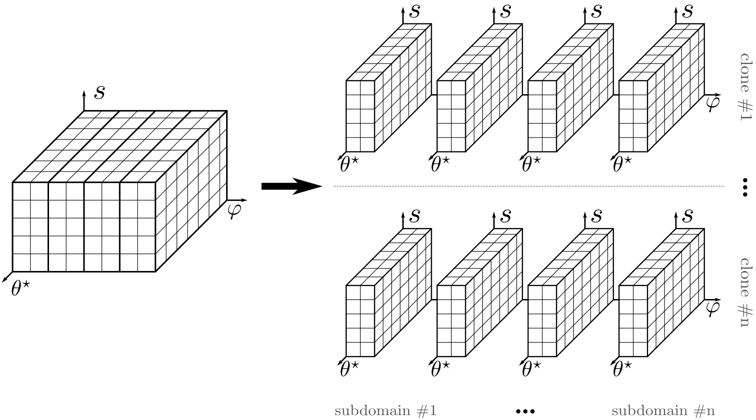
- Global gyrokinetic PIC code:
  - Equations derived from variational formulation with consistent ordering [Tronko, 2017]
  - Ad-hoc or MHD equilibrium
  - Electromagnetic perturbations
  - Different field solver options (long wavelength approximation, Padé approximation, or all orders)
  - Different gyro-averaging options ($\langle \nabla \phi \rangle$ or $\nabla \langle \phi \rangle$)
  - Multiple gyrokinetic species
  - Fixed or adaptive number of Larmor points
  - Drift-kinetic, adiabatic or hybrid electrons
  - Inter- and intra- species collisions
  - Heat sources
  - Strong flows
  - Advanced diagnostics

... with various numerical features

- Numerical features:
  - Variational formulation of field equations with finite element B-splines up to third order
  - Control variate schemes
  - Electromagnetic cancellation problem in Ampère's law solved with enhanced control variate or pullback scheme [Mishchenko, 2014]
  - Runge-Kutta of fourth order time integrator
  - Magnetic coordinates, straight-field-line
  - Field-aligned Fourier filter
  - Noise control (Krook operator, coarse graining, quadtree)
  - Original parallelization: 2 levels of MPI (domain decomposition and cloning)
  - New parallelization: hybrid MPI+OpenMP or MPI+OpenACC

MPI parallelization scheme

- 1D domain decomposition plus domain cloning:



- Reduce/broadcast operations between clones
- All-to-all (parallel data transpose and particle move) and neighboor (guard cells) communications between subdomains

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- Data structures
  - Structure of arrays instead of arrays of structure
  - Pack variables for host-to-device memory transfers

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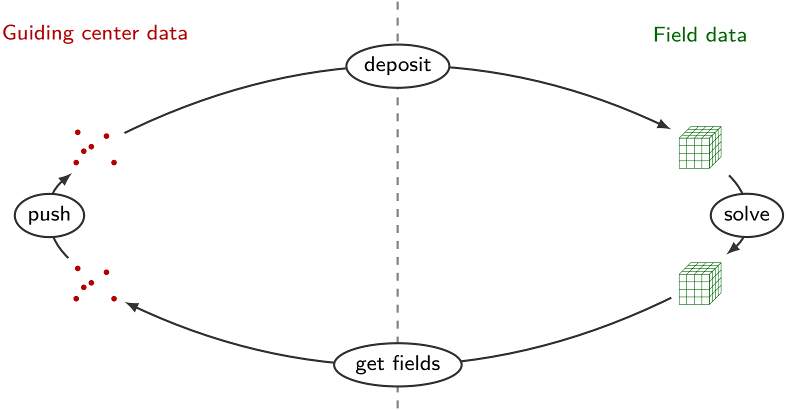

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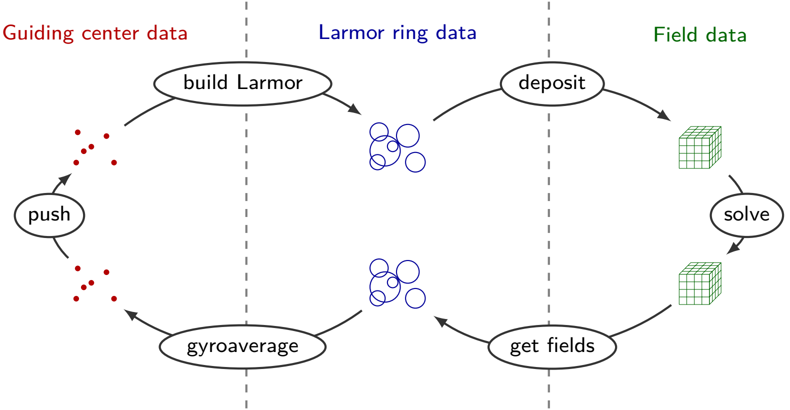
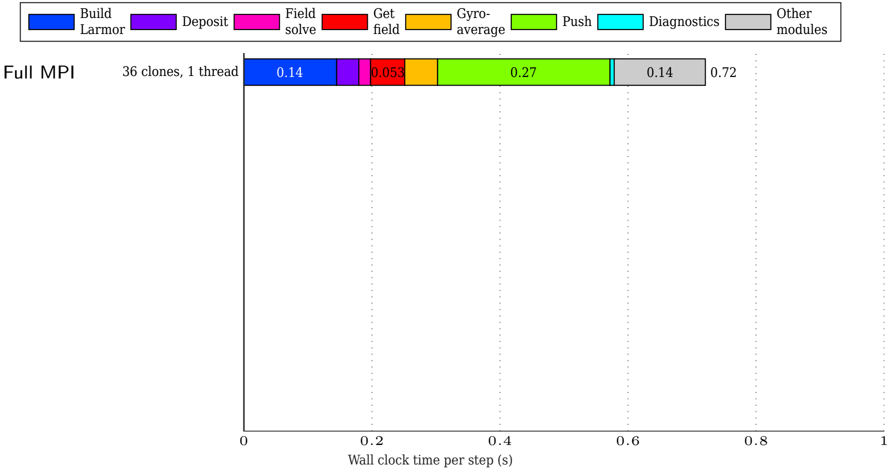


MPI+OpenMP

- Single node simulations with 10^6 ions (4 Larmor points each), 10^6 electrons, and $128 \times 32 \times 4$ cubic splines, on Broadwell CPU (2×18 cores, 2.1GHz)



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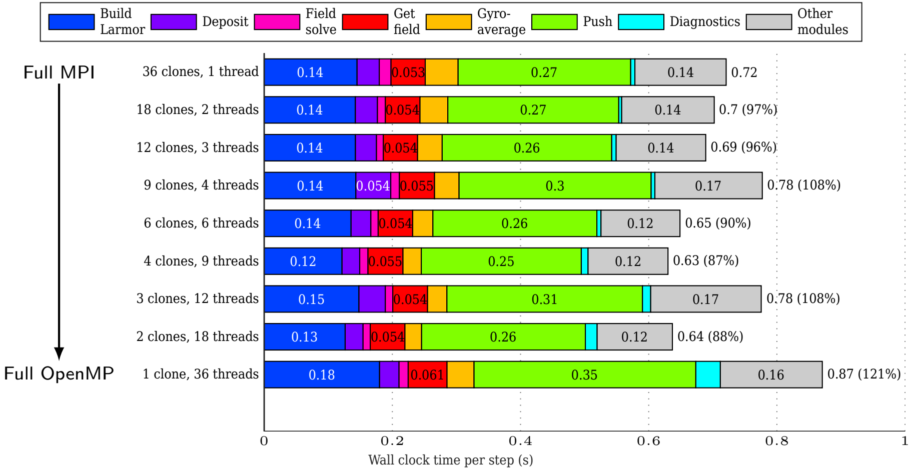

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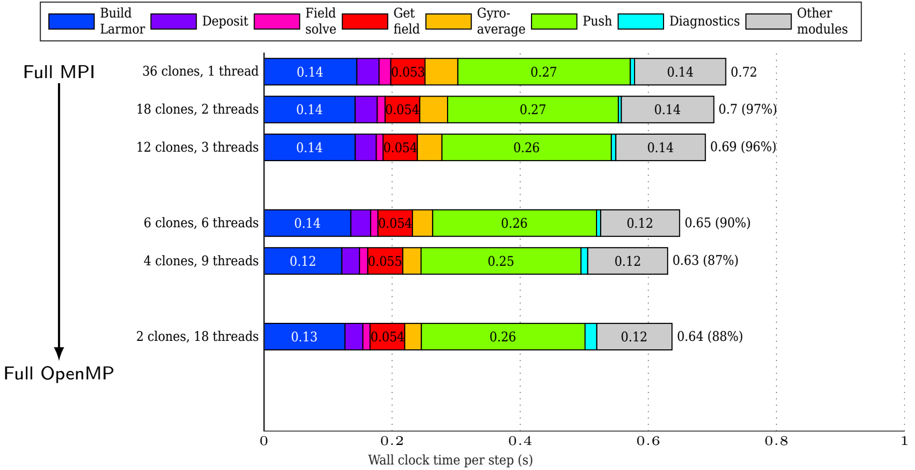

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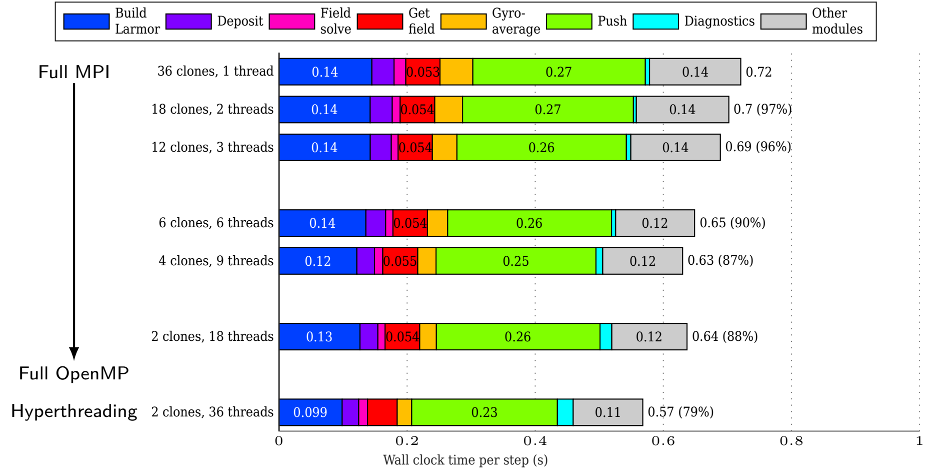

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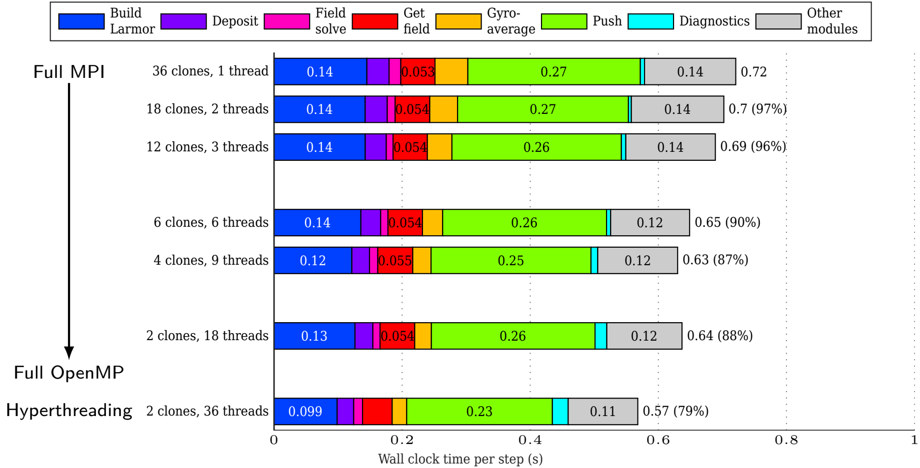

- Up to 20% speed-up by filling sockets with OpenMP threads

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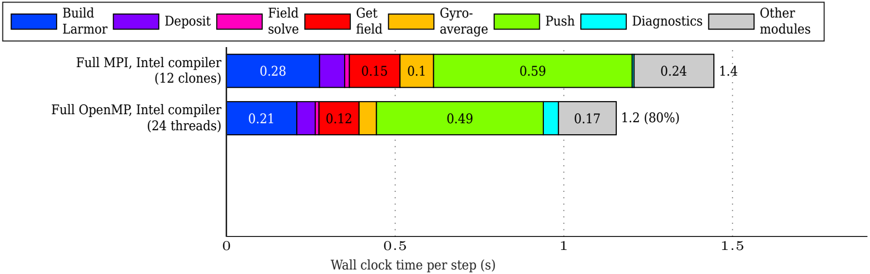

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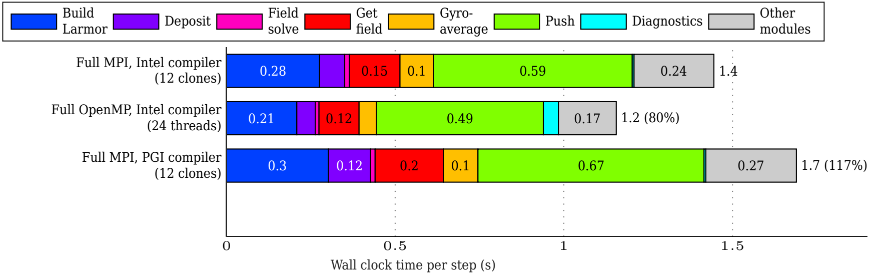

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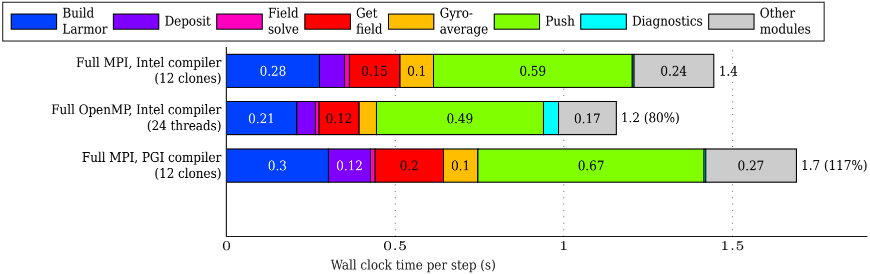

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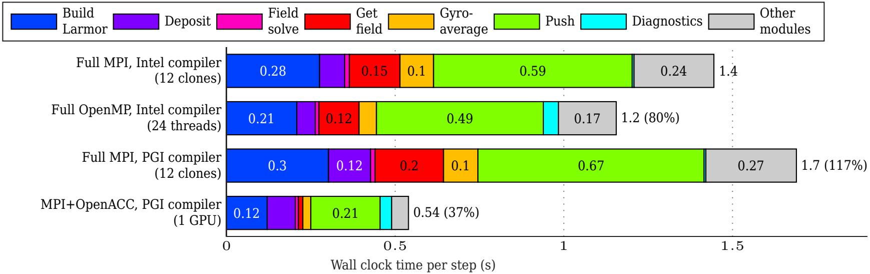

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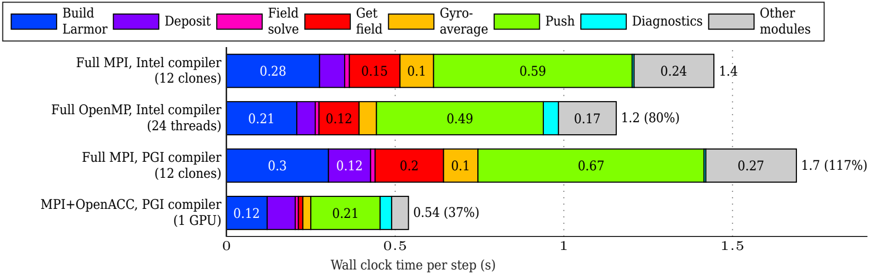

- PGI compiler ∼20% slower than Intel
- MPI+OpenACC version ∼2.7 times faster than MPI only, and ∼2.2 times faster than MPI+OpenMP

Architecture comparisons

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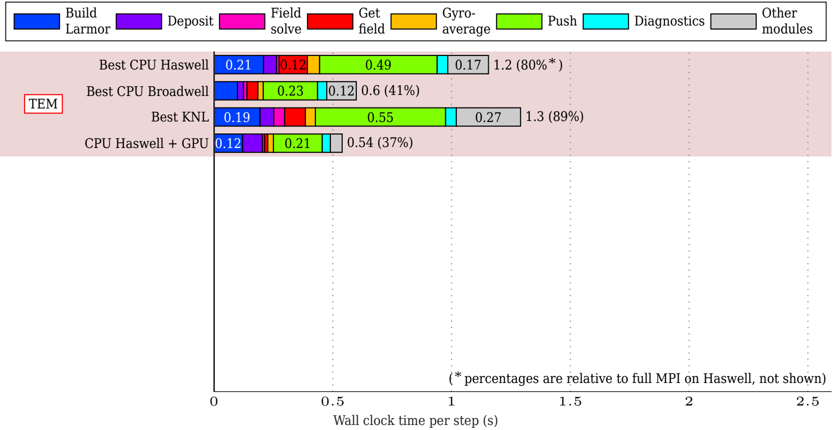
- Different physics (electro-static or -magnetic, adiabatic or kinetic electrons, adaptive number of Larmor points, ...) with similar particle and cell resolutions



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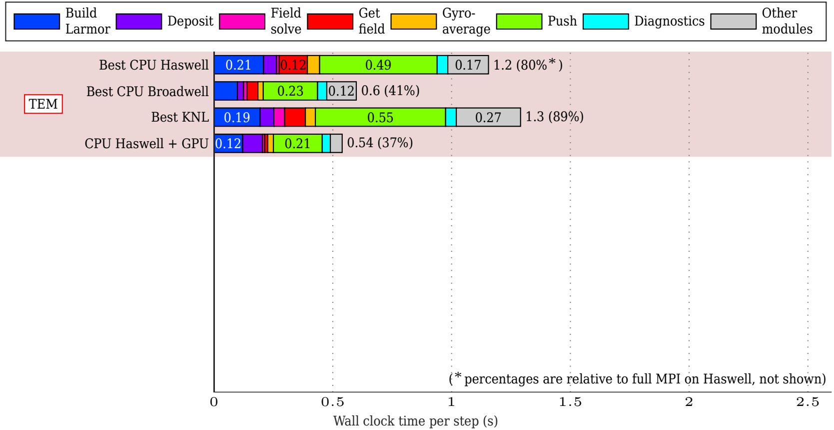

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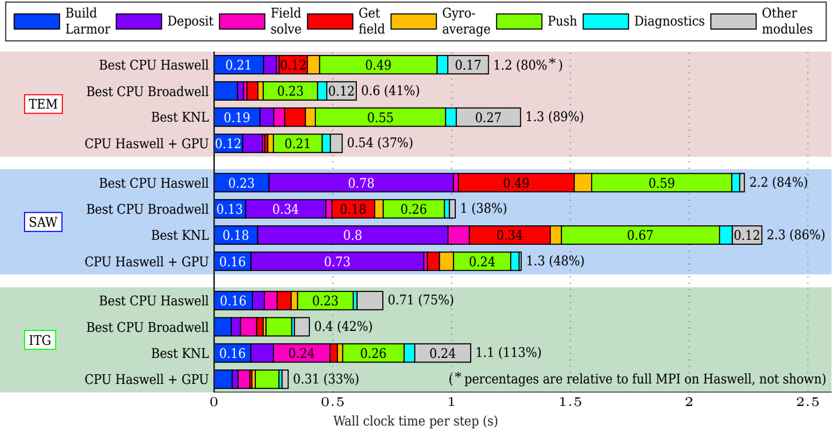

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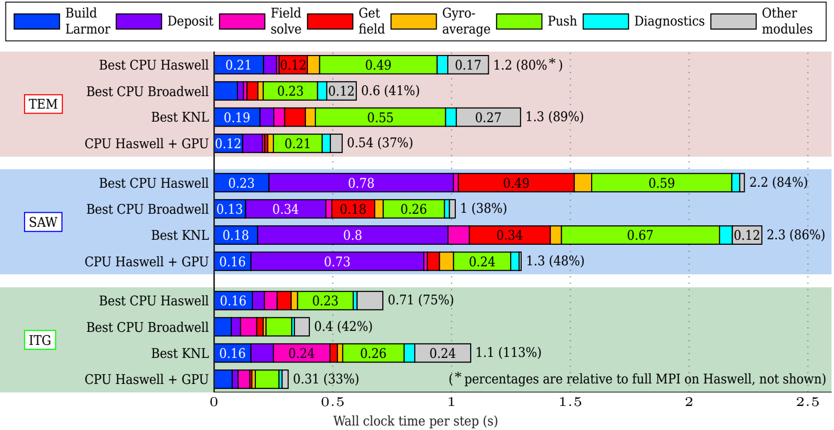
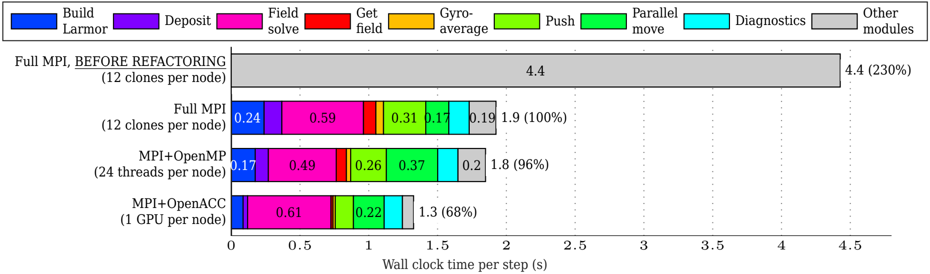


- KNL (64 cores, 1.3GHz) performance similar to Haswell CPU
- Weaker GPU performance for SAW due to control variate iterations on CPU
- GPU performance similar to Broadwell CPU
- Exact factors are case-dependent

Application to production run

- ITG production run on 256 nodes with $256 \cdot 10^6$ ions (4 Larmor points each) and $256 \times 512 \times 256$ cubic splines



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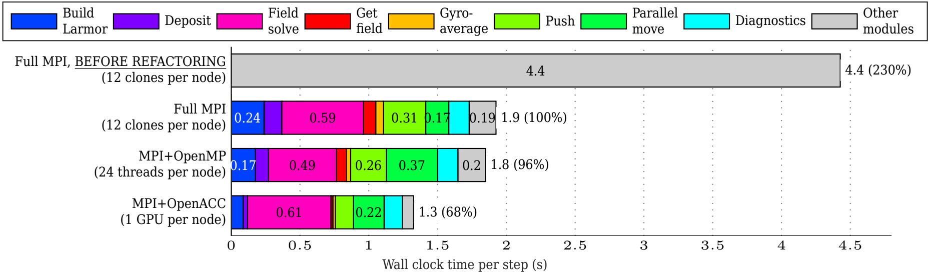

- Timings of communication-bound stages (field solver and parallel move) become non-negligible.
- Multithreaded versions bring less speed-up than on sinle node because they do not improve inter-node communication.
- Full MPI version already 2.3 times faster than before refactoring.

Conclusion

- Achievements:
  - Single code making efficient use of different architectures
  - Good compromise between efficiency, ergonomy, and "future-proofness" (flexibility to accomodate for new physics and new architectures)
- Future work:
  - Turn on sorting when particle-to-field operations are significant
  - Reduce amount of communications in solver

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