Best Practice Identification, Dissemination, and Implementation

Accelerating PIC Simulations on Multicore and Manycore Systems

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Introduction

• GTC-Princeton (GTC-P) → *highly scalable 3D particle-in-cell (PIC) code* used for studying micro-turbulence transport in fusion systems (tokamaks)
• Successfully *ported and optimized on a wide range of multi-petaflops platforms worldwide* at full or near-full system capability: See (Figure 1)
• Code portability aided by fact GTC-P is *not critically dependent on any third-party libraries.*

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Why is GTC-P of significant general interest in HPC R&D ?

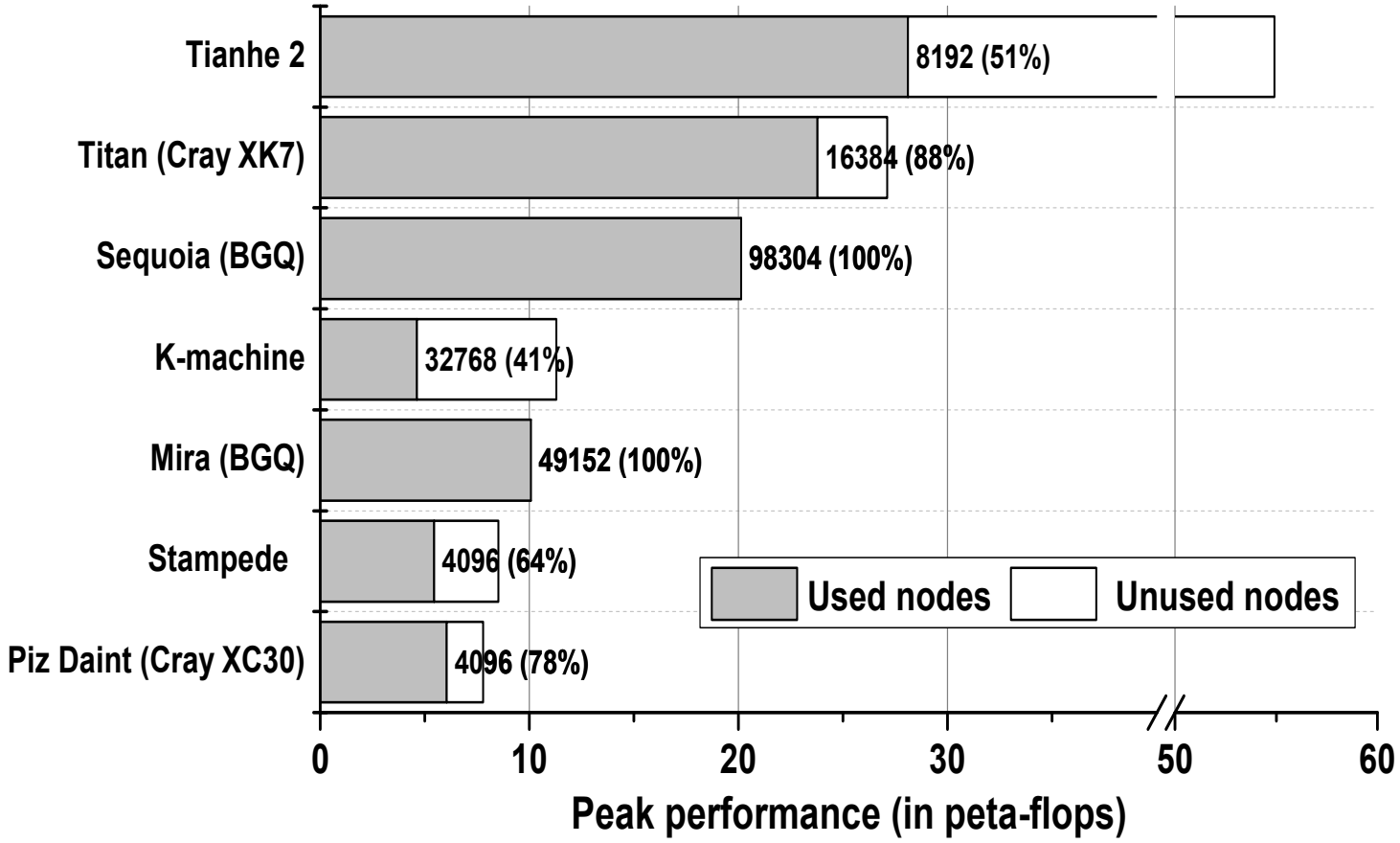

Figure 1: The GTC-P particle-in-cell (PIC) code has been ported to and optimized on a broad range of leading multi-petaflops supercomputers worldwide. Percentage indicates fraction of overall nodes utilized.

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Recent GTC-P Success Story

The R&D approach in GTC-P involves *deployment of a representative modern multi-dimensional particle-in-cell (PIC) code on a large variety of world leading computational platforms*. We highlight various strategies employed to optimize performance, maximize parallelism, leverage accelerator technology, and enable portability across diverse architectures (See Figure 2)

- 2D domain decomposition plus particle decomposition for increasing scalability
- Choice of data layout for maximizing data reuse
- Hybrid Programming models
- Leveraging GPU and Xeon Phi accelerators
- Enabling Portability across different platforms

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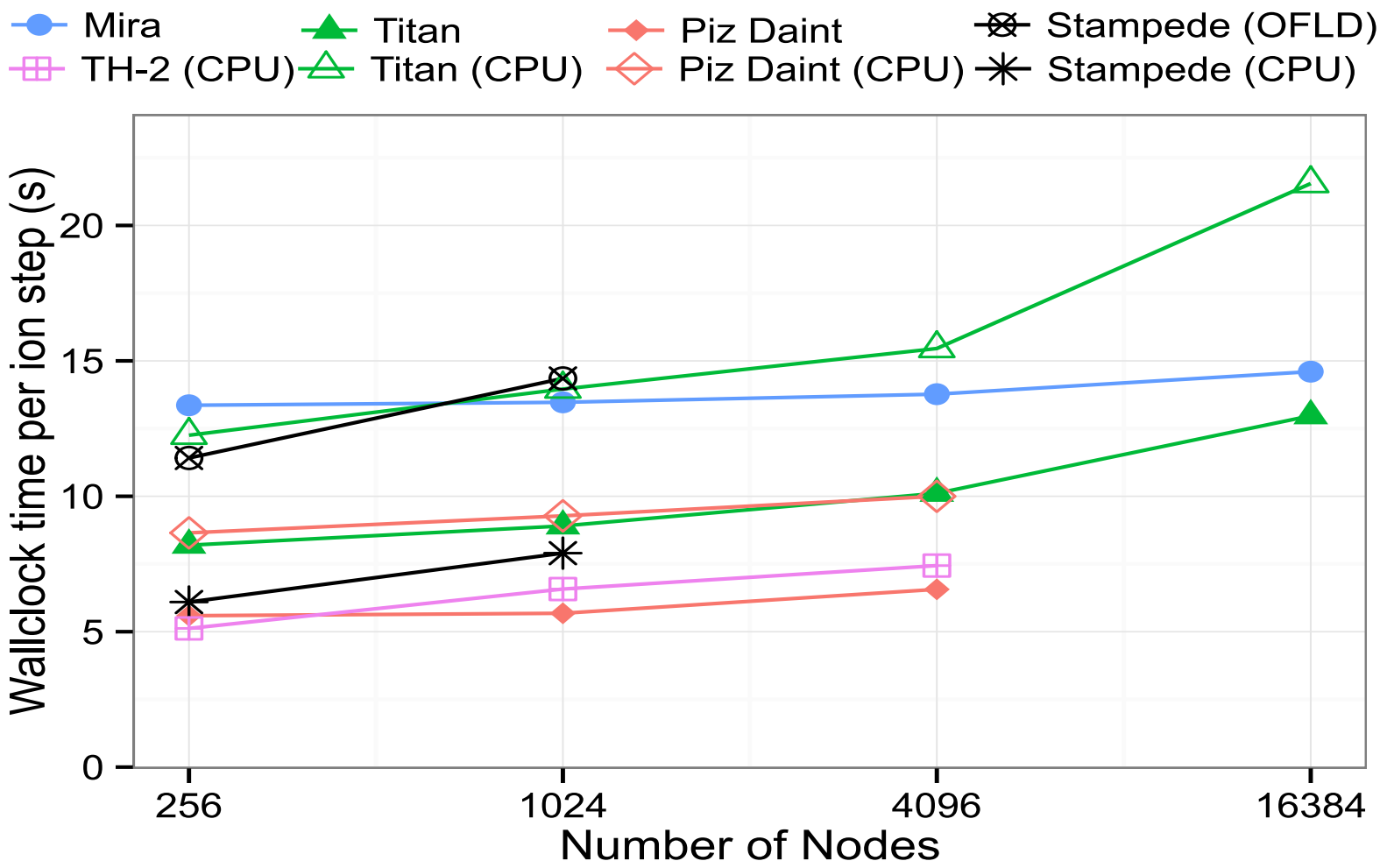

Figure 2: GTC-P code weak scaling performance using a fixed size problem per node across a wide variety of systems.

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Objectives for PRAC: Services Provided

• Overall Goal: Leverage experiences and lessons learned from development of GTC-P on a variety of leading supercomputers worldwide (including NSF's "Blue Waters" and "Stampede") to contribute to all seven categories in the PAID program "Improvement Method Enabler (IMEs)".
• Specific Focus: Accumulate, create, and apply "best practices" for efforts in service of Blue Waters application teams in:

→ *Developing applications that effectively utilize multicore and Many-core systems, maintaining a single code with appropriate interfaces for multiple architectures;*

→ *Explore directives-enabled GPU kernels (e.g., using Open ACC and/or OpenMP4) to improve portability & share with BW-applications teams to help inform their work planning activities*; and

→ *Lowering the threshold for efforts needed to re-engineer BW-applications to improve usage of accelerators/many-core.*

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