Symplectic Structure-Preserving Particle-in-Cell Whole-Volume Simulation of Tokamak Plasmas to 111.3 Trillion Particles and 25.7 Billion Grids

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ABSTRACT

We employ our recently developed explicit 2nd-order charge-conservative symplectic electromagnetic particle-in-cell (PIC) scheme in the cylindrical mesh to simulate the whole-volume magnetic confinement toroidal plasmas on the new Sunway supercomputer. From a large-scale simulation of magnetized toroidal plasma with 111.3 trillion particles and 25.7 billion grids, we have obtained a sustained performance exceeding 201.1 PFLOP/s (double precision) with the fastest iteration step achieving 298.2 PFLOP/s (double precision). For

the first time, unprecedented high resolution evolution of 6D electromagnetic fully kinetic plasmas based on 2D equilibrium profiles from Experimental Advanced Superconducting Tokamak (EAST) and designed operation state of China Fusion Engineering Test Reactor (CFETR) are presented, and edge micro-instabilities can be investigated directly. This shows the possibility to study crucial problems and phenomena in the magnetic confinement toroidal plasma directly using the symplectic electromagnetic fully kinetic PIC method on world's leading supercomputers.

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1 JUSTIFICATION FOR ACM GORDON BELL PRIZE

We employ our recently developed symplectic structure preserving fully kinetic Particle-in-Cell scheme in cylindrical coordinates and have measured 95.6% weak scaling efficiency and a sustained performance of 201.1 PFLOP/s using 103,600 nodes of the new Sunway supercomputer. Simulation of whole-volume tokamak plasma to 1.113×10^{14} particles and 2.57×10^{10} grids is achieved.

2 PERFORMANCE ATTRIBUTES

<i>Category of achievement:</i>	peak performance, scalability
<i>Type of method used:</i>	explicit symplectic
<i>Results reported on the basis of:</i>	whole application excluding I/O
<i>Precision reported:</i>	double precision
<i>System Scale:</i>	measured on full-scale system
<i>Measurement Mechanism:</i>	timers, FLOP count

3 OVERVIEW OF THE PROBLEM

3.1 Development of Tokamaks

Faced with the coming energy crisis, human beings have a common dream to seek an infinite and clean energy for sustainable development. Tokamak [2], initially conceptualized in the 1950s, is currently the most promising magnetic confinement fusion (MCF) device that can eventually provide clean, safe and nearly unlimited fusion energy in the future. Its basic idea is using strong toroidal magnetic field to confine high temperature plasmas. The magnetic field configuration of a Tokamak is shown in Fig. 1(a). Inside a Tokamak magnetic field, the particles are moving along the trapped orbit or passing orbit, and if no dissipation they will be bounded in the device permanently. Development of Tokamaks and the product they achieved is summarized in Fig. 1(b). It can be seen that inside a Tokamak which can actually output energy, the plasma needs to be heated to above 100 million degrees Kelvin in order to significantly exceed the fusion triple product condition, while the magnet surrounding the plasma requires very low temperature to maintain the superconductivity. Such huge temperature and pressure gradient will drive various micro-instabilities and turbulences that significantly degrade the confinement performance. To overcome this difficulty, the device is required to be very large, and international efforts have been made to build the next generation International Thermonuclear Experimental Reactor (ITER) [3]. Devices with similar plasma parameters, China Fusion Engineering Test Reactor (CFETR) [47] and SPARC [30], are also proposed for supplement of ITER and demonstration of power plant validation. Behaviours of fusion (burning) plasmas, energetic particles and how the high power auxiliary heating techniques designed for these large Tokamaks can effect the burning plasma are under investigation. While in another aspect, methods to suppress the turbulence are also worthy to be tried since they may decrease the cost. All these studies and attempts need high fidelity simulation of kinetic plasmas at extreme scales.

3.2 Particle-in-Cell method applied to Tokamak physics

The Particle-In-Cell (PIC) method proposed in 1960s [6, 13, 19] is a powerful tool for studying plasmas and beam physics. It directly solves the evolution of charged particles coupled with electromagnetic fields, governed by the following equations:

$$\frac{\partial \dot{\mathbf{x}}_{sp}}{\partial t} = \frac{q_s}{m_s} (\mathbf{E}(\mathbf{x}_{sp}) + \dot{\mathbf{x}}_{sp} \times \mathbf{B}(\mathbf{x}_{sp})), \quad (1)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad (2)$$

$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \sum_{s,p} q_s \dot{\mathbf{x}}_{sp} \delta(\mathbf{x} - \mathbf{x}_{sp}), \quad (3)$$

where dielectric constant and permeability in the vacuum are set to 1 for simplicity, $\mathbf{E}$ and $\mathbf{B}$ are electromagnetic fields, q_s , m_s , $\mathbf{x}_{sp}$ and $\dot{\mathbf{x}}_{sp}$ are the charge, mass, position and velocity for the p -th particle of species s . For many crucial but complex problems in magnetic confinement plasmas, such as the micro-instabilities in the edge plasma, lower hybrid current drive, ion cyclone resonant heating, and energetic particle induced instabilities, the first-principle based electromagnetic 6D (i.e., 3-dimensional space and 3-dimensional velocities) fully kinetic PIC method is desired, and usually these problems require simulations of whole-volume or near whole-volume plasmas. Understanding these problems can help explain experimental phenomena, design better plasma configuration and optimize auxiliary heating methods. This is especially useful for now because at present, modeling for next generation devices such as ITER and CFETR requires integrating higher-fidelity multiscale whole volume plasma models into simulations [7], as illustrated in Fig. 1(c). It will be significantly beneficial if we find a way by simulation that can reduce even 1% total cost of the devices.

In this work, we present large-scale fully kinetic simulations of whole-volume Tokamak plasmas using our recently developed explicit 2nd-order charge-conservative symplectic electromagnetic PIC scheme for cylindrical regular meshes [41]. For the first time, the whole-volume plasma based on equilibrium of existing Tokamak (e.g., Experimental Advanced Superconducting Tokamak, EAST [37]) experiment and designed operation state of future Tokamaks (e.g., CFETR) are numerically investigated directly using the most basic charged particle coupled with electromagnetic field plasma model. With the help of world's leading new Sunway supercomputer and good scalability of the scheme, we can simulate the evolution of unprecedented $N_R \times N_\psi \times N_Z \times \text{NPG} = 3072 \times 2048 \times 4096 \times 4320$ toroidal plasmas with 1.113×10^{14} marker particles, where N_R , N_ψ , N_Z , N_{total} and NPG are the number of grids in the axial, toroidal, height directions and number of marker particles per grid, respectively. A sustained performance of 3.724×10^{13} particle push per second (201.1 PFLOP/s) and peak performance of one iteration step of 298.2 PFLOP/s are measured. As examples, we demonstrate the simulated high resolution of edge instabilities based on equilibrium profiles of EAST and designed CFETR H-mode plasmas.

4 CURRENT STATE OF THE ART

Due to the multiscale nature of the magnetic confinement plasmas, it is very difficult to apply the 6D PIC method for simulating

Figure 1: The development of modern and future Tokamaks requires whole-volume simulations. (a) A schematic diagram of Tokamak magnet configuration and trapped particle orbit inside that magnetic field. (b) The achievement of fusion product of Tokamak devices, including 3 projection of planned devices (ITER, CFETR and SPARC) in the future, where Q_{DT} is the ratio between fusion power and heating power in a deuterium-tritium plasma. $Q_{DT} > 1$ means the fusion power is larger than the external heating power and $Q_{DT} = \infty$ is the self-sustained burning condition or the well known Lawson criterion. Data are collected from Refs. [38, 44]. (c) The development of whole volume simulation of Tokamak plasmas, including the physical model, spatial-time range, and the computing resource available at that time. Designing and modeling of Tokamak operations with larger in size and higher parameters requires whole volume simulation of plasmas using high fidelity models that contains more physical processes.

Table 1: Performance of PIC simulators with different algorithms on top supercomputers. Here the abbreviations GK, FK, NPG, and CG represent gyrokinetic, fully kinetic and number of sampling particles per grid, and Sunway core group, respectively. Note that for GK PIC methods, solving GK Poisson or Ampere equations is usually implicit and may not have good scalability. The symplectic FK PIC scheme used in this work consumes about 5000 FLOPs when calculating the pushing and current deposition for one particle, while conventional non-symplectic Boris-Yee based FK PIC schemes this number is around 250 (VPIC [8])–650 (PIConGPU [45]) FLOPs.

Work	Year	Algorithm	Precision	Machine	# CPU cores	# GPUs	NPG	Performance (particle push/s)
GTC [46]	2019	GK, δf	fp32	Summit	40.8K	5568	100K	5×10^{11}
GTC-P [36]	2013	GK, δf	fp32	Mira	524K	-	500	1.34×10^{11}
GTC-P [35]	2019	GK, δf	fp32	Piz Daint XC30	32.8K	4096	100	4.2×10^{10}
ORB5 [28]	2021	GK, δf	fp64	Piz Daint XC50	24.6K	2048	37.3	7.1×10^8
ORB5 [28]	2021	GK, δf	fp64	Summit	180K	24.6K	37.3	2.9×10^9
VPIC[8]	2008	FK, full-f	fp32	Roadrunner	122K	-	32.1K	1.5×10^{12}
VPIC2.0[4]	2021	FK, full-f	fp32	Sierra	79.2K	7.2K	-	2.4×10^{12}
PIConGPU[11]	2019	FK, full-f	fp32	Summit	202K	27.6K	25	1.62×10^{13}
This work	2021	FK, full-f, symplectic	fp64	New Sunway	621.6K (CGs)	-	4320	3.725×10^{13}

the evolution of whole-volume magnetic confinement plasmas. In this section, we introduce existing works focus on the PIC simulation on large-scale clusters, including gyrokinetic PIC simulation of toroidal plasmas and conventional 6D fully kinetic PIC simulations on top supercomputers. A summary including the present work is listed in Tab. 1.

4.1 Gyrokinetic PIC simulations

The space-time span of the whole-volume plasma evolution is very large, and directly using fully kinetic PIC schemes will cost huge amount of computational resources. To increase the maximum allowed time-step and hence reduce the computational cost, people introduced gyrokinetic (GK) PIC method [12, 15, 24, 25] in which

the particles are modelled as guiding centers to investigate low frequency turbulence problems in Tokamaks [25]. It should be noted that in GK simulations not just the gyro-averaging approximation or gyro-center coordinate transform is adopted. Some other techniques such as the magnetic static approximation, parallel magnetic vector potential assumption, GK Poisson equation [24] and GK Ampere equation [15] for approximations of Maxwell equations are also included. This is because in strongly magnetized plasmas, not only the gyromotion, but also the plasma oscillation, electromagnetic modes, or even Alfvén modes will limit the time-step. GTC [46], GTC-P [35, 36] and ORB5 [28] are commonly used GK codes for large-scale plasma simulations on recently developed supercomputers. The performance behavior of GK PIC methods may be very different compared to fully kinetic PIC ones since they could involve implicit Poisson solvers, we still list them in Tab. 1 for reference.

In spite of the great success of gyrokinetic simulations, it was pointed out recently [20, 26] that the ordering assumption of the gyrokinetic theory [14, 23] is not always valid in certain circumstances [34]. Another issue is that solving Poisson equation in gyrokinetic codes does not scale well on large clusters, which may limit the parallel performance. These problems restrict the accuracy and speed of gyrokinetic simulations on modern large heterogeneous supercomputers.

4.2 Fully kinetic PIC simulations

Fully kinetic (FK) PIC methods directly solves the Vlasov-Maxwell or Vlasov-Poisson equations. Previously they were mainly used in simulating high-frequency physics such as the laser-plasma interactions and magnetic reconnections. A commonly used FK PIC scheme is the Boris-Yee scheme [5, 19], which is locally explicit and thus can have very good scalability on large clusters. A typical implementation, VPIC [8, 9], uses an improved version of this scheme. VPIC also employs a variety of Single Instruction Multiple Data (SIMD) intrinsics to fully utilize the floating point performance provided by modern processors. Recently people focus on porting conventional FK PIC schemes to GPU-based clusters, for example the development of VPIC2.0 [4] and PIConGPU [10, 11]. These FK electromagnetic PIC schemes are usually memory bandwidth bounded since one push and current deposition process in the Boris-Yee scheme only requires 250-650 floating point operations (FLOPs) [8, 45], while updating a particle in the memory need at least 24/48 bytes read and 24/48 bytes write for the case of fp32/fp64 precision.

4.3 Symplectic PIC methods

The fast development of supercomputers is making it possible to conduct 6D electromagnetic fully kinetic PIC simulations of whole-volume magnetic confinement plasmas. However, conventional 6D PIC algorithms do not possess the long-term accuracy and fidelity, which means even if unlimited computing resource exist, long-term results obtained by these algorithms are not reliable. To tackle this challenge, a series of structure preserving geometric PIC methods [16, 22, 29, 32, 39–43] are developed to overcome the numerical dissipation (e.g., self-heating [18]) problem of conventional PIC

methods. Based on discrete exterior calculus (DEC), Whitney interpolating form, canonical or noncanonical symplectic integrators, these PIC methods preserve discrete symplectic 2-form exactly during the iteration and thus have unparalleled long-term conservation property that conventional PIC methods do not have. Such conservation properties have been proved in practice [17, 22, 27, 43].

The symplectic structure-preserving PIC schemes are developed since 2012; however to our knowledge, the present work is the first one that investigates the performance optimizations and parallel scalability of the symplectic PIC simulation of whole-volume Tokamak devices on leadership supercomputers. Compared to the commonly employed Boris-Yee scheme, the 2nd-order charge-conservative symplectic PIC scheme used in this work requires more arithmetic operations for the push and current deposition process (about 5000 FLOPs according to our measurement) of one particle. So on most modern clusters the symplectic PIC scheme will become computationally intensive and more FLOP performance can be achieved. There are also other advantages to use symplectic PIC scheme in simulating magnetic confinement plasmas even if the memory bandwidth limitation on conventional Boris-Yee PIC schemes did not exist. First is that the grid size can be chosen to be much larger than the Debye length λ_D and no numerical instability is observed. Secondly the time-step can be also chosen as $\Delta t \Omega_{pe} \sim 1$, while usually in conventional explicit PIC methods $\Delta t \Omega_{pe} < 0.2$ for the accuracy reason [33]. Lastly there is no numerical dissipation in the symplectic PIC scheme, which means we can run the simulation for very large number of time-steps as long as we need without worrying about the conservation property of the algorithm.

5 INNOVATIONS REALIZED

5.1 Algorithm innovation

In this work, we employ our recently developed state-of-the-art method, i.e., explicit 2nd-order charge conservative symplectic structure preserving electromagnetic PIC scheme for cylindrical coordinates. Detailed updating rule can be found in the Appendix B of Ref. [41]. It is based on modern geometric techniques such as DEC and Whitney interpolating forms in cylindrical coordinates, and variational symplectic or noncanonical Hamiltonian splitting integrators. Compared to conventional PIC schemes, our new symplectic PIC scheme exactly preserves the discrete noncanonical symplectic 2-form of the Hamiltonian charged particle-electromagnetic field system. Numerical errors of invariants such as total energy and momentum can be therefore bounded by a small number. As examples, the numerical self-heating problem in conventional PIC simulations is automatically eliminated in our symplectic PIC simulations, and the number of simulation time-steps can be chosen as much larger than that in conventional Boris-Yee based PIC schemes because no numerical dissipation is involved.

The algorithm is implemented in the *SymPIC* (<https://github.com/JianyuanXiao/SymPIC/>) which focuses on implementing structure preserving PIC schemes with both high performance and portability on modern large-scale heterogeneous clusters. The *SymPIC* code mainly consists of following modules: a scheme interpreter

for loading configuration files, field solver, particle pusher and current deposition calculator, particle sorter, I/O module and the initializer for initial conditions. The workflow of *SymPIC* is shown in Fig. 2.

Figure 2: The workflow of *SymPIC*.

5.2 Multi-platform code generation

To increase the power efficiency and computing density, heterogeneous architectures are more preferable when building large supercomputing systems. Many of these heterogeneous architectures have their own programming APIs or even languages. For example, the Summit supercomputer utilizes an CPU+Nvidia GPU architecture, the Sunway TaihuLight supercomputer is built based on Sunway manycore processors, and the Tianhe-2A supercomputer employs an heterogeneous architecture with CPU+NUDT Matrix Accelerator. Developing applications to support all these heterogeneous platforms simultaneously could be challenging, but not impossible since all these heterogeneous cluster nodes have similar Management-Worker (MW) structures, therefore can be programmed with a consistent MW programming model. In particular, the conventional multi-core CPU can be also viewed as a special type of MW node.

To achieve multi-platform portability on heterogeneous clusters, we have developed a Domain Specific Language (DSL) named ParallelScheme to Many Core (PSCMC, <https://github.com/JianyuanXiao/pscmc>) (PSCMC) that can describe the MW programming model and corresponding code generator. It is Turing complete and hence can be employed to implement arbitrary parallel algorithms. Currently it supports code generation backends of serial C, OpenMP, CUDA, Sunway Manycore (SWMC) Athread interface, OpenCL, HIP, NUDT Matrix Accelerator Interface (MAI), and SYCL.

Our *SymPIC* code is implemented with PSCMC, therefore supports all the aforementioned parallel platforms, even including future CPU+AMD GPU and CPU+Intel GPU based clusters by using the PSCMC HIP and SYCL backends.

As an example, we demonstrate the multi-platform code generation procedure of the *SymPIC* code in Fig. 3. Firstly, some complex

mathematical formulas used in *SymPIC* such as the particle pushing scheme and weighting functions are derived by using the Maxima computer algebra system [1] from the variation of discrete action integral as required by the symplectic method. This will make it easy to ensure the correctness of the tedious implementation of these complex formulas. Then the *SymPIC* PSCMC source code will be compiled into platform-specific code by using the PSCMC compiler, which is a multi-pass source-to-source compiler written in the scheme programming language. Its basic idea is dividing the compiler to a series of small source-to-source compiler passes, each of which performs a much easier task [21, 31]. Some features such as a small type-inference system and a parallel-for loop vectorization procedure are also added.

Except for the good portability of codes to modern heterogeneous supercomputers, it also has many other advantages to use the PSCMC (or other similar DSLs, if any) for implementing numerical algorithms. Firstly, new MW heterogeneous platforms can be supported by adding corresponding code generation backends to PSCMC. According to our tests, to add support for one C programming language based heterogeneous programming environment such as OpenMP, CUDA, HIP, SWMC and MAI, only 100-200 lines of scheme code is required, which is significantly smaller compared to directly porting applications to that platform, especially when the application is large and complicated. Even for the more complicated OpenCL and SYCL, a new backend needs less than 400 lines of scheme code which is still very few. Secondly, once we change an existing part or add a new algorithm to the application implemented with PSCMC, they will support all the parallel platforms automatically. Last but not least, the PSCMC compiler supports generating pure serial C codes, which is more convenient for debugging purpose. Once the generated serial C code behaviors as expected but a parallel code does not, it means that errors have occurred during parallelization and thus can provide hint for debugging.

We should clarify that to achieve state-of-the-art performance, it is required to consider vendor provided specific optimizations or unique features other than the MW programming model can describe. For example, asynchronous direct memory access (DMA) on Sunway CPUs, shared memory/local memory on CUDA, HIP, OpenCL and SYCL, shuffle instructions on CUDA and HIP supported GPUs, and SIMD and prefetch instruction on modern CPUs. In the PSCMC codes, all these optimizations can be implemented by using macros similar to that in the Common Lisp. These macros can generate platform-specific code based on the choice of backends, and generate equivalent codes for other platforms.

5.3 Process-level and thread-level parallelizations

To achieve high scalability on large-scale heterogeneous parallel computer systems, the key is to provide enough parallelism and balanced task partition. In *SymPIC*, the simulation domain is decomposed into small computing blocks (CBs) using the Hilbert space filling curve. An example of a 16×16 mesh grid decomposed into 4×4 CBs by the 2nd-order Hilbert curve is shown in Fig. 4(a). In this example, there are three MPI processes in total, and the

Figure 3: Typical code generation and compiling procedure of an application written in PSCMC. Here we use the *SymPIC* code as an example.

Figure 4: Parallelization scheme and optimizations in *SymPIC*: (a) process level parallelization; (c) branch-avoiding optimization; (d) locations of stored particles and grids; (e) auto-vectorization; (f) dual buffering optimization.

computing blocks are almost evenly distributed in the whole communication domain. Further, computing blocks can be distributed using strategies considering non-uniformly distributed particles and the performance difference of computing devices (e.g., CPU and GPU). Considering that particles can move to another grid or another CB during the simulation, it is necessary to get particles sorted to achieve better performance. Therefore we design a two-level particle buffer system to handle this issue. For each grid in

the CB, a continuous memory block with fixed size, i.e., grid buffer, is allocated to store positions and velocities of particles. Typically the grid buffer size should be larger than the average number of particles in that grid. For each CB, an additional memory block with fixed size, i.e., CB buffer, is allocated to sort particles or to store particles when overflow happens for some grids inside that CB. In this two-level particle buffer system, most of the particles will be stored in the memory contiguously and located in the same

nearest grid. So many advanced techniques, such as SIMD/SIMT optimization and asynchronous DMA in Sunway computing processing element (CPE), can gain more performance improvement.

We employ the 2nd-order of Whitney interpolating form in *SymPIC*. Therefore the knowledge of field values at $4 \times 4 \times 4$ grid points around that particle and two ghost grid layers are required for pushing one particle, as shown in Fig. 4(a). As an example, the actual grid buffer for storing field values of a 2D CB with size 4×4 will be 8×8 . Therefore, when neighboring CBs update the grid data in parallel, there will be write conflicts. Adding lock can solve this problem, but this method has non-negligible time overhead on various hardware platforms. In order to generate code suitable for various platforms, *SymPIC* stores a data copy of ghost grids together with the local grids for each CB. This method also introduces costs when maintaining the consistency of the ghost grids. To maximize the performance, the simulation domain needs to be divided into more computing blocks to increase the parallelism, but each computing block needs to contain enough cells to keep less ghost area data copies.

To balance this trade-off, we implement two strategies for handling particle motions in the thread-level parallelism. The first CB-based task assignment strategy is that particles in one CB is calculated by one CPU thread (or CUDA thread-block, OpenCL workgroup, etc.), in this case there will be no conflicts between two different threads. But when the number of CBs in one process is small and not be a multiply of the number of hardware threads, the hardware resources will not be fully exploited. To overcome this issue, we have also implemented the second grid-based task assignment strategy. In this one all grids in one process will be most evenly distributed to CPU threads, so it will have better performance when the number of CBs is small compared to the first strategy. But the drawback is that an additional buffer for storing the current is required to eliminate the write conflict of each thread and an extra current accumulation procedure is called after the particle push. According to our tests when the number of CBs is a multiply of the number of CPU threads, using the first strategy the overall speed will be about 10-15% faster than using the second one.

5.4 Particle sorting and auto-vectorization

For modern high performance CPUs, SIMD units are usually equipped to further increase the computing density. Unfortunately until now, according to our tests modern compilers (gcc-9 and clang-10) cannot generate assembly codes that can effectively use the SIMD instruction for long loops, even with some directives such as `#pragma omp simd` are given. To use these SIMD units in modern CPUs more efficiently, we design a specific syntax structure `parafor` to tell the PSCMC compiler to automatically vectorize a specific for loop using specified SIMD intrinsics. The basic idea is grouping each N_S statement then translate them into equivalent single statement using SIMD intrinsics (see Fig. 4(d)), where N_S is the length of SIMD vector (e.g., in the double precision case, for AVX2 $N_S = 4$, for AVX512 and Sunway 512bit SIMD $N_S = 8$). It currently supports all SIMD intrinsics that are supported by gcc and clang. It can also specify an SIMD mask variable to deal with the last turn of the `parafor` loop where the number of rest iterations could be smaller than the length of SIMD vector.

Most of computing time in *SymPIC* is consumed in the particle pusher and current accumulation procedure. For particles inside one grid cell, the above procedure can be calculated together, we thus use the `parafor` to automatically vectorize it. In this version of implementation, each turn N_S particles are calculated together. It should be noted that particles will move from one grid cell to another in one time-step. To achieve better performance, the key is to eliminate branches in the algorithm. As an example, we demonstrate the calculation of interpolated electric field in one direction without introducing branch in Fig. 4(b). As we have previously mentioned, particles are mostly stored in the nearest grid point of their coordinates. So in one grid with indices j , the actual coordinate of the particle x_{sp} should comply $j-0.5 < x_{sp} \leq j+0.5$, as illustrated in Fig. 4(c). Here to simplify the notation, we let the grid size $\Delta x = 1$. There are two kinds of particles, i.e., $x_{s1} > j$ and $x_{s2} \leq j$. Suppose we have $x_{1,2} = x_{s1,2} - \text{floor}(x_{s1,2})$, then their interpolation coefficients should be calculated by two divergent functions, W_l^+ and W_l^- . But we can also calculate it by a predicate vector ($x_{s1,2} > j$), i.e.,

$$W_{j+l}(x_{s1,2}) = \text{vselect}(x_{1,2} > j, W_l^+(x_{1,2}), W_l^-(x_{1,2})).$$

If a computing device does not support the `vselect` instruction, it can be fallen back to

$$W_{j+l}(x_{s1,2}) = (x_{s1,2} > j) \times W_l^+(x_{1,2}) + (x_{s1,2} \leq j) \times W_l^-(x_{1,2}).$$

Calculations of magnetic field and current can be done in a similar manner. At this point, all branches are eliminated.

Surprisingly, it should be noted that as long as the relation of $j-1 \leq x_{sp} \leq j+1$ holds, we can still correctly calculate the particle motion and current using the above procedure. Therefore the calling of the sort procedure could be less frequently than that of the calculating procedure. This further increases the overall performance a lot because the particle sorting procedure is memory bandwidth bounded. The maximum allowed number of time steps without sorting depends on the maximum speed of charged particles. Typically for electrons with thermal speed $V_{th,e} = 0.05c$ and $\Delta t = 0.5\Delta x/c$, we can do particle sorting once for every 4 particle pushes. One more thing, because all supported target of *SymPIC* share the same source code, the above branch-eliminated particle pushing code is automatically applied to the GPU version, which also improves the performance on GPUs.

5.5 Memory-efficient optimizations

The data required for the particle pusher and current accumulation procedure primarily includes the interpolation grids of electromagnetic fields and current, and the coordinates and velocities of the particles inside each grid in a CB. On the new Sunway supercomputer, Each CPE of the many-core CPU, SW26010Pro, has 256KB scratchpad memory (SPM) space, we configure it as 224KB local data memory (LDM) and 32KB cache. Therefore the LDM size is significantly larger than that of its predecessor SW26010 which only has 64KB LDM. This allows us to put more frequently accessed data into the LDM. In this work, electromagnetic fields and current in one CB are put in the LDM if the size of CB including ghost grids is smaller than a configurable number of grid points.

In the computing kernel, particles are accessed sequentially and only once, so it is not necessary to stay in the LDM for a long time. The Sunway CPE provides an asynchronous DMA transfer mechanism to quickly load such data. To hide the memory transfer latency, the particles are grouped and loaded to two buffers in the LDM, buffer A and buffer B, as shown in Fig. 4(e). Each particle group can hold up to 32 particles. The calculation of each group is divided into two steps. In the first step, half of the group, i.e., 16 particles in buffer A are processed while the DMA_PUT operation of the particle group in buffer B is executed. And in the second step, the computation for the other 16 particles in buffer A is carried out while performing DMA_GET operation for loading a new particle group into buffer B. After the two steps, the pointers of buffer A and buffer B are swapped to start another cycle of the dual buffering process. On SW26010Pro, for the symplectic structure preserving PIC scheme employed in *SymPIC*, the time used in data transfer between LDM and main memory is smaller than that is consumed on the calculations of particles, therefore the memory transfer latency can be completely hidden.

5.6 I/O optimizations

In *SymPIC*, I/O mainly occurs when saving field results and checkpoints. During large-scale simulations, writing huge amount of data into a single file will be very time-consuming. To utilize the bandwidth provided by the filesystem in modern clusters, we design a lightweight I/O library that supports arbitrary number of I/O groups. According to our tests, in the large scale simulation of CFETR plasma with 262,144 MPI processes on the new Sunway supercomputer, 250 GB output data per I/O time-step can be written to the global filesystem in 1.74–10.5 seconds when using 8192 I/O groups. The new Sunway supercomputer is also equipped with a smaller but fast object-based storage system for storing temporary data. We use it to output the checkpoints. During the above CFETR plasma simulation, one checkpoint has the size of 89TB. Loading or saving one such checkpoint using 32768 I/O processes will cost about 130 seconds. Usually the checkpoint is set to be updated every 1.5–2hrs, therefore the I/O for checkpoints takes approximately 1.8% to 2.4% of the total simulation time.

6 HOW PERFORMANCE WAS MEASURED

6.1 System and environment

As the successor of Sunway TaihuLight, the new Sunway supercomputer consists of more than 103,600 SW26010Pro heterogeneous many-core processors. The architecture of SW26010Pro CPU is shown in Fig. 5. Each chip of the SW26010Pro processor contains 6 core groups (CGs). Each CG is the most basic unit that implements the manager-worker many-core architecture. In a CG, there is a management processing element (MPE) serving as the manager core and 64 computing processing elements (CPEs) arranged in an 8×8 grid acting as worker cores. As compared to its predecessor, SW26010, the upgraded CPE in SW26010Pro has 256KB scratchpad memory (SPM) and supports wider 512 bit SIMD operations. The SPM on CPE can be configured as either user-controlled local data memory (LDM) or hardware cache for automatic data buffering. The software stack on the new Sunway supercomputer includes a

customized MPI library, compilers that support C, C++ and Fortran, vendor-provided library named Athread for the thread-level parallel programming on CPEs, and a job scheduler which supports management of over 40 million heterogeneous cores.

Figure 5: The architecture of SW26010Pro many-core processor equipped in the new Sunway supercomputer.

6.2 Application description

All tests in this article are performed on a problem that describes the toroidal plasma with following parameters unless explicitly specified,

$$v_{th,e} = 0.0138c, \quad (4)$$

$$\Delta_R = \Delta z = 102.9\lambda_{De}, \quad (5)$$

$$\Delta_\psi = 3.43 \times 10^{-5} \text{ rad}, \quad (6)$$

$$\Delta_\psi R_0 = \Delta R, \quad (7)$$

$$\Delta_t = 0.5\Delta_R/c = \frac{0.75}{\omega_{pe}} = \frac{0.59}{\omega_{ce}}, \quad (8)$$

$$\mathbf{B}_{ext}(R) = \frac{R_0 B_0}{R} \mathbf{e}_\psi. \quad (9)$$

where $v_{th,e}$ is the thermal velocity for electrons, $R_0 = 2920\Delta R$ is the location of the left boundary of the simulation domain, $\omega_{ce} = B_0 e/m_e$, ω_{pe} and λ_{De} are the electron plasma frequency and Debye length. These parameters can be used in simulations of whole-volume Tokamak plasmas that can resolve gyro-motion of ions. To reduce the numerical noise, the number of marker particles per grid for electrons is set to 1024. For performance testing cases, ions are set to be fixed.

6.3 FLOPs measurement

To achieve high-fidelity simulations, *SymPIC* needs to use the double precision floating point numbers as required by the structure preserving symplectic PIC scheme. Since the generated code is very large, manually counting all double-precision arithmetic instructions in the assembly code is impractical. Instead, we use the following two methods to obtain FLOPs performance:

- (1) collecting the number of double-precision arithmetic operations by using the hardware performance monitor provided by the vendor of new Sunway supercomputer,
- (2) and using the Linux perf tool to measure the double-precision arithmetic operations on an Intel Xeon Gold 6142 computer

by running the same OpenMP version of our code with AVX-512 optimizations.

Result from the first method indicates that for calculating one particle, approximately 5.4×10^3 FLOPs is required, while the corresponding number reported by the second method is around 5.1×10^3 . This slight discrepancy originates from the difference of these two platforms, and is relatively small. In this work we use the first method to calculate the FLOPs results.

7 PERFORMANCE RESULTS

7.1 Portability test on various platforms

Since our *SymPIC* code can be ported to many heterogeneous computing platforms, it is interesting to examine its performance on them. We list the single-node or single-device results of *SymPIC* to compare the performance of *SymPIC* on some typical platforms in Tab. 2. In the table, we summarize the running time of each PIC iteration loop to simulate a 3D computational domain with each grid containing 1024 marker particles initially. Each CB has a shape of $4 \times 4 \times 4$ and the order of 3D Hilbert curve is chosen as the maximum value allowed by the memory. “Push” means the number of million particle pushes per second for a PIC iteration step without the sort procedure, “All” means the average Push performance if one sort procedure is called every 4 PIC iterations. It can be seen from the table that the *SymPIC* code performs well on all the tested heterogeneous computing devices, clearly indicating that *SymPIC* is able to efficiently support heterogeneous computing across different architectures. In particular, with 390 cores and 512bit SIMD FPU, SW26010Pro performs the best amongst these platforms.

Table 2: Performance comparison of *SymPIC* on various heterogeneous platforms. Here N.C. means the number of cores. On CUDA GPUs, we record one GPU SM unit as one core, and the 64bit*32 SIMD means each thread-block contains 32 CUDA threads. The TH2A node consists two 12-core E5-2692v2 CPUs and two 128-core Matrix-2000 accelerators, so the number of cores is 280.

Hardware	ISA	Arch.	SIMD	N.C.	Push	All
Gold 6248	x64	CSL	AVX512	40	220	192
E5-2680v3	x64	Haswell	AVX2	24	69.8	65.1
Hi1620-48	ARMv8	TS-V110	ASIMD	96	101	95.4
Phi-7210	x64	KNL	AVX512	64	114.7	106.6
Titan V	-	GV100	64bit*32	80	98.3	87.0
Tesla A100	-	GA100	64bit*32	108	224	194.4
TH2A node	-	IVB+MT	AVX	280	140.8	114.3
SW26010Pro	SW	SW	512bit	390	344	261.1

7.2 Many-core acceleration on SW26010Pro

To further investigate the performance improvement of *SymPIC* on the new Sunway platform, we compare the speed-up results using optimization techniques introduced in this work. In each CG of SW26010Pro, most computing performance is provided by the 64 CPEs. Therefore to achieve high performance on the new Sunway supercomputer, it is crucial to effectively use all these CPEs. Figure 6 shows the performance evaluation of *SymPIC* considering various optimizations employed in this work. The running time of

the MPE-only version generated by the PSCMC serial C code backend is used as a baseline.

Figure 6: The running time of different subroutines in each PIC iteration loop using 8 CGs for computing problems with the configuration same to the portability tests. Here MPE, CPE, SIMD, MSS and D&L represent the MPE-only version, the initial CPE version generated by PSCMC, the 512 bit SIMD vectorized version, the multi-step sort version, and the final version including dual buffering and LDM optimizations, respectively.

For the MPE-only version, the most time-consumption kernel in *SymPIC* is the particle push and current calculator, which takes 91.8% wall-time. The corresponding CPE version directly generated by PSCMC is 39.6 times faster, and 3.09 more times faster when using the PSCMC automatic SIMD loop optimization. Finally when the dual buffering and the LDM optimizations are applied, we gain another 2.26 times performance boost. In total a 277.1 times acceleration is achieved using the fully optimized CPE kernel compared to the original MPE-only version for particle push and current calculation.

The particle sorting procedure is memory bandwidth bounded, thus directly using the PSCMC generated CPE code only has a 9.5 times performance boost. However because our particle push and current calculator allows particles that are not exactly located in the corresponding grid, the number of required sort procedure can be reduced. In this case we sort once for each 4 PIC iteration time-steps, which immediately results a 4 times acceleration. So the overall many-core acceleration of particle sort procedure is 38.0.

Combining all the optimization techniques listed above, we obtain a final 138.4 times acceleration of our symplectic PIC scheme using the Sunway CPEs.

7.3 Strong scaling test

In the strong scaling tests, we set the number of grids in each direction and the number of particles as in Tab. 3. The size of one CB is $4 \times 4 \times 6$ and the sort procedure is called every 4 iteration steps, the I/O module of *SymPIC* is disabled, and only the PIC iteration time is recorded. Performances are calculated using the wall time for iterating 100 time-steps.

The measured strong scalability results are shown in Fig. 7. Here for problem A, because the number of CBs is 2^{24} , so when the total numbers of CPEs are larger than 2^{24} (for 524,288 and 616,200 CGs)

Table 3: Number of grids and particles for the strong scaling test, where two scales (A and B) of problems are tested.

Scale	N_R	N_ψ	N_z	# marker particles	Number of CGs
A	1024	1024	1536	1.65×10^{12}	616200
A	1024	1024	1536	1.65×10^{12}	524288
A	1024	1024	1536	1.65×10^{12}	262144
A	1024	1024	1536	1.65×10^{12}	131072
A	1024	1024	1536	1.65×10^{12}	65536
A	1024	1024	1536	1.65×10^{12}	32768
A	1024	1024	1536	1.65×10^{12}	16384
B	2048	2048	3072	1.32×10^{13}	616200
B	2048	2048	3072	1.32×10^{13}	524288
B	2048	2048	3072	1.32×10^{13}	262144
B	2048	2048	3072	1.32×10^{13}	131072

Figure 7: Sustained performance of the strong scaling test.

we use the grid-based discretization strategy for updating particles, which increases the total computational complexity but provides more parallelism; for other cases we still use the CB-based discretization strategy. It can be seen that *SymPIC* has a good strong scaling efficiency of 91.5% when the number of CGs increases from 16,384 to 262,144. For 524,288 and 616,200 CGs because of the adoption of the grid-based discretization strategy the parallel efficiency drops to 73.0% and 70.4%. But it is still better than using CB-based one because in these cases the particle push procedure using CB-based discretization strategy cannot gain performance compared with using 262,144 CGs. For problem B which is around 8 times larger than problem A, scaling from 131,072 to 524,288 CGs leads to a parallel efficiency of 97.9%. For the largest case of 616,200 CGs we have tested both CB-based and grid-based strategies and find that the CB-based one performs better. So the overall strong scaling efficiency for problem B from 131,072 CGs (8,519,680 processor cores) to 616,200 CGs (40,053,000 processor cores) is 87.5%.

7.4 Weak scaling test

In the weak scaling tests, the configurations of the problem is shown in Tab. 4, and the experiments are done following similar rules as in the strong scaling tests. The test results are presented in Fig. 8, from which it can be seen that the performance of *SymPIC* increases nearly perfectly as the number of CGs and problem scale

Table 4: Number of grids and particles for weak scaling tests.

N_R	N_ψ	N_z	# marker particles	Number of CGs
64	64	96	4.03×10^8	8
128	128	192	3.22×10^9	64
256	256	384	2.58×10^{10}	512
512	512	768	2.06×10^{11}	4096
1024	1024	1536	1.65×10^{12}	32768
2048	2048	3072	1.32×10^{13}	262144
3072	2048	4096	2.64×10^{13}	621600

Figure 8: Sustained performance of the weak scaling test.

increases. We obtain a weak scaling efficiency of 95.6% from 8 CGs (520 processor cores) to 621,600 CGs (40,404,000 processor cores), corresponding number of particles and grids are from 4.03×10^8 to 2.639×10^{13} and 3.93×10^5 to 2.577×10^{10} , respectively.

7.5 Peak performance test

Table 5: Number of grids and particles for the peak performance test.

N_R	N_ψ	N_z	# marker particles	Number of CGs
3072	2048	4096	1.113×10^{14}	621600

For peak performance measurement, we use the simulation parameters displayed in the Tab. 5. We use the the plasma of $3072 \times 2048 \times 4096$ grids with 4320 electron marker particles per cell, and the simulation is performed on 103,600 nodes (40,404,000 processor cores) of the new Sunway supercomputer. The sorting procedure is called every 4 time-steps. For one iteration time-step without sort procedure, 2.016 second is cost which resulting a peak performance of 298.2 PFLOP/s in double precision. For each 4 time-step iterations, additional 3.890 second is cost to call the sort procedure, therefore the average iteration time for one time-step is 2.989 second and we can obtain a sustained performance of 201.1 PFLOP/s in double precision. The code reaches a final 3.724×10^{13} sustained particle push per second performance.

8 IMPLICATIONS

8.1 Application results

Using the optimized *SymPIC* code on the new Sunway supercomputer, we have managed to simulate two whole-volume Tokamak H-mode plasmas using 2D fluid equilibrium profiles.

The first one is based on the equilibrium of H-mode plasma generated in the shot-86541 of EAST, its resolution is $N_R \times N_\psi \times N_z = 768 \times 256 \times 768$ with $\Delta R \approx 0.55\rho_i$ where ρ_i is the gyro-radius of thermal ions. Here electron-deuterium plasma is used, the mass ratio between electron and deuterium is 1 : 200, and in the center of the plasma NPG of electrons and ions are set to 768 and 128. In this case 32768 CGs (2,129,920 processor cores) are used and the total simulation time is 1 day (including I/O, checkpoint and rerun due to the arrangement of job queue). A total 3.4×10^5 time-steps are simulated, and the 3D density distribution of last time-step can be shown in Fig. 9 (a). From Fig. 9 (a) we can see that at the edge of the plasma belt-structure unstable modes occurs. Structures of unstable modes with different toroidal mode number n can be also demonstrated in Fig. 9 (b).

For the second case, we generated a plasma based on the fluid equilibrium of H-mode burning plasma in a designed fusion operation mode of CFETR. Its resolution is $N_R \times N_\psi \times N_z = 1024 \times 512 \times 1024$ with $\Delta R \approx 1.5\rho_i$ where ρ_i is the gyro-radius of thermal deuteriums. This plasma contains 7 species of charged particles, which are electrons with mass of 73.44 times the real mass of electrons, deuteriums, tritiums, thermal heliums, argons, fast deuteriums with a center temperature of 200keV, energetic fusions generated alpha particle with a center temperature of 1081keV. Corresponding NPG in the center for each species are set to 768, 52, 10, 10, 10, 80. In this case 262,144 CGs (17,039,360 processor cores) are used and the total simulation time is 1.5 days (including I/O, checkpoint, and rerun due to the node failure). A total 4.6×10^5 time-steps are simulated, and the 3D pressure of last time-step can be shown in Fig. 10 (a). It is clear that the designed CFETR H-mode plasma is much more stable than the EAST H-mode plasma, and we can barely see the unstable modes from the density perturbation. To demonstrate the unstable modes at the edge, we also draw the magnetic perturbation of different toroidal mode number n in Fig. 10 (b). For the first time, the unprecedented whole-volume fusion plasma containing deuteriums, tritiums, heliums, fast deuteriums and fusion generated energetic alpha particles are directly simulated with the electromagnetic fully kinetic PIC method. Because of the excellent conservation property of the symplectic PIC scheme, we can investigate the low frequency phenomena in the plasma without worrying about the numerical dissipation problems.

8.2 Symplectic structure-preserving electromagnetic fully kinetic PIC simulation of whole-volume Tokamak plasmas

We have implemented and optimized our recently developed symplectic structure-preserving PIC scheme for cylindrical regular meshes on the Sunway many-core architecture. With the help of world's leading new Sunway supercomputer, unprecedented large-scale

Tokamak plasmas can be directly simulated by using the fully kinetic PIC method. This enables the numerical investigation of many crucial physical and engineering problems for whole-volume Tokamak plasmas using the fully kinetic model. Compared to gyrokinetic PIC schemes used previously, the present method is based on a more fundamental Vlasov-Maxwell physical model. A typical advantage in Tokamak physics is that in our simulations the self-consistent electric field is naturally formed in the 2D equilibrium of plasma, and it evolves nonlinearly with the evolution of the 6D whole-volume plasma. This is crucial in Tokamak plasmas especially when investigating edge related physics since at that place radial electric fields are strong and has close relation to $\mathbf{E} \times \mathbf{B}$ drift motion, instabilities and turbulences.

In this work, the most unstable mode of whole-volume Tokamak plasma can be obtained and nextly we can try to find a way to suppress it, which may serve as a guidance to improve the performance of future large Tokamaks such as ITER and CFETR, and eventually accomplish more economical controlled fusion energy. Other important problems such as wave heating and current drive, energetic particles induced instabilities, energy deposition of fusion alpha particles can be also investigated. Before the machines are actually built, fully kinetic simulation results will also support and improve their designs.

8.3 *SymPIC* and PSCMC on other platforms

Though this work mainly focus on the optimization of *SymPIC* on the Sunway many-core platform, it should be noted that *SymPIC* has excellent portability because the employment of PSCMC and most performance optimizations introduced in this work can be directly applied to other hardware architectures. For example the automatic SIMD loop optimizer can generate any SIMD intrinsics that supported by gcc or clang and hence boost the performance on common high-performance CPU platforms, while the reduction of number of sort procedure will also reduce the memory bandwidth requirement on conventional multi-core CPU and GPU nodes. These optimizations have already applied to *SymPIC* on other heterogeneous platforms.

The PSCMC can be also employed to implement other applications or algorithms that can beneficial from the management-worker programming model. It makes single-source code that supports all present world's leading supercomputers possible. The most exciting part is that writing a PSCMC backend to support new heterogeneous platform requires very small effort. In most cases it is much easier than directly porting the applications to support that platform. While platform specific optimizations can be also implemented by writing macros in PSCMC source code. This means both high efficiency and high portability can be achieved together, which is highly desired for today's high performance computing developments. We have open sourced both *SymPIC* and PSCMC, and hope that our efforts will be of common interest to the community of PIC simulations and Tokamak plasma physics.

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Figure 9: Simulation results of the EAST H-mode plasma. (a) The 3D density distribution of a turbulence state. (b) The unstable mode structures of electron density with different toroidal mode number n . Here the contour shows mode distribution normalized by the initial core density n_0 .

Figure 10: Simulation results of the designed CFETR H-mode plasma. (a) The 3D pressure distribution of an instability increasing state. (b) The unstable mode structures of B_R with different toroidal mode number n . Here the contour shows mode distribution normalized by 1 Tesla. It can be seen that the unstable mode also occurs at the edge of the plasma.

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