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Implementation of 2D Domain Decomposition in the UCAN Gyrokinetic Particle-in-Cell Code and Resulting Performance of UCAN2

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Abstract. The massively parallel, nonlinear, three-dimensional (3D), toroidal, electrostatic, gyrokinetic, particle-in-cell (PIC), Cartesian geometry UCAN code, with particle ions and adiabatic electrons, has been successfully exercised to identify non-diffusive transport characteristics in present day tokamak discharges. The limitation in applying UCAN to larger scale discharges is the 1D domain decomposition in the toroidal (or z-) direction for massively parallel implementation using MPI which has restricted the calculations to a few hundred ion Larmor radii or gyroradii per plasma minor radius. To exceed these sizes, we have implemented 2D domain decomposition in UCAN with the addition of the y-direction to the processor mix. This has been facilitated by use of relevant components in the P2LIB library of field and particle management routines developed for UCLA's UPIC Framework of conventional PIC codes. The gyro-averaging specific to gyrokinetic codes is simplified by the use of replicated arrays for efficient charge accumulation and force deposition. The 2D domain-decomposed UCAN2 code reproduces the original 1D domain nonlinear results within round-off. Benchmarks of UCAN2 on the Cray XC30 Edison at NERSC demonstrate ideal scaling when problem size is increased along with processor number up to the largest power of 2 available, namely 131,072 processors. These particle weak scaling benchmarks also indicate that the 1 nanosecond per particle per time step and 1 TFlops barriers are easily broken by UCAN2 with 1 billion particles or more and 2000 or more processors.

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Key words: Gyrokinetic simulation, particle-in-cell method, massive parallelization.

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1 Introduction

Nonlinear gyrokinetic equations which describe complex plasma dynamics over time scales that are long compared to the Larmor or gyro motion perpendicular to the ambient magnetic field have come to play a fundamental role in our understanding of the confinement-time behavior of strongly magnetized plasmas [1]. Gyrokinetic particle-in-cell (PIC) codes which solve these gyro motion-averaged equations have proven to be powerful tools to study anomalous plasma transport in magnetic confinement devices such as tokamaks [2]. Among these, global codes [3–8] which cover the whole plasma cross-section or the entire plasma minor radius the short way around the torus, the other direction being the toroidal one along the major radius the long way around the torus, aim to describe at once plasma behavior throughout the whole device. Such global codes became feasible with the advent of the fully nonlinear δf method of Parker and Lee [9]. With this method, the perturbed part of the distribution function, δf, over its static equilibrium counterpart f_0, which defines the total distribution function as $f = f_0 + \delta f$, is followed dynamically using discrete particles over a fixed background grid where the plasma response fields are evaluated. The δf description does however entail evolving in time and space weights which represent the fraction of phase space ($\delta f/f$) associated with every gyrokinetic particle in addition to velocities and positions as in conventional full f PIC codes. These global codes have become practical as physics tools with their massive parallelization for multi-processor mainframes such as the very recent Cray XC30 Edison at the National Energy Research Scientific Computing Center (NERSC) in the US or the IBM MareNostrum III at the Barcelona Supercomputing Center (BSC) in Spain.

The UCAN gyrokinetic code, developed jointly at the University of California at Los Angeles (UCLA) and University of Alberta, Canada, hence the acronym, is one of these early global codes to use PIC methods [10] to solve the gyrokinetic equations with only electrostatic effects included [4, 5]. The electrons are treated (analytically) as being adiabatic in UCAN and only the kinetic ions are followed as particles. UCAN has the added oddity that it uses Cartesian coordinates, as opposed to magnetic field-following coordinates, which encompass the toroidal geometry with the z-direction accounting for the toroidal one and the x-y plane representing the poloidal cross section. The plasma cross-section is however circular in that plane with the particles excluded from occupying the region outside the limit circle whose radius is specified as a certain, suitably large, number of ion gyroradii. Because of that exclusion, the boundary conditions for the field quantities can be taken as periodic without apparent deleterious effects. Spatial operations in UCAN are handled using finite differences on the fixed background Cartesian grid and Fast Fourier Transforms (FFTs) where appropriate, such as when solving the gyrokinetic Poisson equation to calculate the electrostatic potential from the gyrophase-averaged, or gyroaveraged for short, ion density accumulated from the particles. Along with the gyrokinetic Poisson equation, the equations of motion of the particle ions actually used in UCAN have been given in detail in Kniep [11]. We remark that a three-level predictor-corrector scheme is utilized for the time advance of the velocities, positions,