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Abstract — *Integrated modeling (IM) of present experiments and future tokamak reactors requires the provision of computational resources and numerical tools capable of simulating multiscale spatial phenomena as well as fast transient events and relatively slow plasma evolution within a reasonably short computational time. Recent progress in the implementation of the new computational resources for fusion applications in Europe based on modern supercomputer technologies (supercomputer MARCONI-FUSION), in the optimization and speedup of the EU fusion-related first-principle codes, and in the*

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development of a basis for physics codes/modules integration into a centrally maintained suite of IM tools achieved within the EUROfusion Consortium is presented. Physics phenomena that can now be reasonably modelled in various areas (core turbulence and magnetic reconnection, edge and scrape-off layer physics, radio-frequency heating and current drive, magnetohydrodynamic model, reflectometry simulations) following successful code optimizations and parallelization are briefly described. Development activities in support to IM are summarized. They include support to (1) the local deployment of the IM infrastructure and access to experimental data at various host sites, (2) the management of releases for sophisticated IM workflows involving a large number of components, and (3) the performance optimization of complex IM workflows.

Keywords — *High-performance computer, infrastructure for integrated modeling, code optimization and parallelization.*

Note — *Some figures may be in color only in the electronic version.*

I. INTRODUCTION

Integrated modeling (IM) of present magnetic fusion experiments, aimed at an improved understanding of the physics of tokamak plasmas and the development of predictive capabilities for future experiments and tokamak designs based on validated physics models, is an important component of the EUROfusion Consortium's mission goals.[1] The EUROfusion strategy in this area includes three main elements: (1) the provision of sufficient computational resources for fusion applications based on the most advanced technology; (2) the support for development of validated advanced first-principle physics codes capable to describe multiscale phenomena within a reasonably short computational time and adaptation of these codes to modern high-performance computer (HPC) architecture; and (3) the integration of the physics codes into a unique IM suite to be efficiently used on a supercomputer.

From 2012 to 2016, the first requirement was successfully addressed within the Broader Approach (BA) activities under the framework of collaboration between Japan and Euratom (Ref. 2). The Computer Simulation Centre was set up within the BA and its computational resources (HELIOS supercomputer) were actively and efficiently used by the European Union (EU) fusion community. Following the shutdown of HELIOS at the end of 2016, EUROfusion took a strategic decision to implement a supercomputer for fusion applications in Europe. A high-level support team (HLST) was established within the European Fusion Development Agreement (EFDA) back in 2009 to address the second requirement, and it successfully continues its activities in providing support with code optimization and parallelization and sharing its expertise with a broad community of developers of first-principle codes for magnetic fusion applications. The third requirement is addressed by a core programming team (CPT) which was also created under EFDA to develop and maintain the European IM infrastructure. These teams include the high-level experts in computational physics, computer science, numerical methods, and high-performance computing. Following the success achieved by the CPT with the IM infrastructure development, which eventually became a prototype for the ITER IM infrastructure, the scope of this EUROfusion team has been recently extended to include support to users of the IM tool on physics and technical issues as well as support to the strategic movement of the EUROfusion modeling activities toward ITER standards. The progress in the implementation of the supercomputer for fusion applications in Europe, in the optimization and speedup of EU theory-based codes to adapt them to modern HPC architecture, and in the development of a basis for integration of physics codes into a centrally maintained suite of IM tools achieved by the EUROfusion HLST (Ref. 3) and CPT is summarized in this paper.

II. EUROfusion COMPUTATIONAL CAPABILITIES (HPC MARCONI-FUSION)

Following the increasing computational needs of first-principle simulations and IM, the growing number of HPC users, success in code optimization, and the ability to scale to a large number of cores, the EU extended its computational capabilities by acquiring a new supercomputer for fusion applications under EUROfusion. This supercomputer, called MARCONI-FUSION, is a dedicated part of a larger supercomputer hosted at the Inter-University Computing Consortium (CINECA) (Bologna) under a EUROfusion Project Implementing Agreement with the National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA)/CINECA.

It consists of two parts: a conventional processor part and a many-cores processor part. The first phase of the conventional part [based on Intel Xeon-Broadwell processors for a total peak performance of 1 petaflop (Pflop)] of this machine has been operational since mid-2016 and its replacement in a second phase [5 Pflop of Intel Xeon-Skylake processors] is now in progress. The accelerated part, in production since the beginning of 2017, consists of 1 Pflop of Intel Knights Landing many-cores processors. The purpose of this partition is to offer EUROfusion users, in continuation of the Intel Knight Corner partition of HELIOS, access to compute nodes that are very efficient for highly parallel and well-vectorized codes. The compute nodes are interconnected by an Intel Omni-Path network with a fat-tree topology with bandwidth performances measured by means of the Intel MPI Benchmark (Fig. 1), and are connected to a high-performance general parallel file system (GPFS) storage system. Thanks to the CINECA Tier-0 Development Roadmap of the HPC infrastructure for the period 2015 to 2020, the EU fusion community takes advantage of HPC resources based on the latest technology generation of processors.

To provide the facility for IM which can run massively parallel codes, a new Gateway is embedded into MARCONI-FUSION hosting the IM tools developed by EUROfusion. A cluster of 24 computer nodes has been configured in a flexible environment, allowing graphical interactive remote sessions and batch job submissions as well. Thanks to a common Omni-Path low latency network, a GPFS storage system, and a portable batch system (PBS) batch queue system, Gateway users can exploit the HPC computing resources of the whole MARCONI. The Gateway software resources are based on the system and application software of MARCONI on which the CPT and Gateway support team have developed an ad-hoc user environment based on a modules tool. The Gateway enables users to perform distributed workflows (WFs), i.e., WFs executing partly on a distributed HPC architecture and partly on the Gateway (for example, the WF for transport-turbulence simulations where the first-principle turbulence simulations can be done on the HPC architecture). For such WFs, specific KEPLER (Ref. 4) actors for launching jobs on the HPC architecture and accessing consistent physical objects (CPO) data remotely through the universal access layer[5] (UAL), as well as a parallel input/output (I/O) extension of the UAL (Ref. 6) were developed.

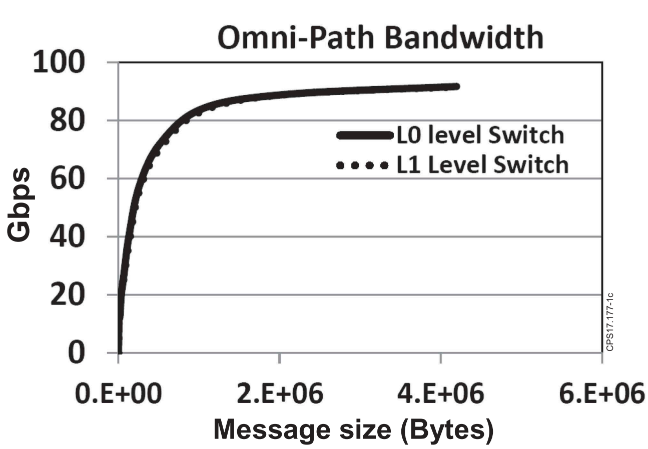

Fig. 1. Ping-pong test for two different level switches implemented on MARCONI's conventional partition.

III. ENABLING EFFICIENT FIRST-PRINCIPLE PHYSICS SIMULATIONS

Progress in the development of fusion theory motivates further development of numerical tools capable of addressing the identified new physics effects. Typically, modeling such effects is computationally challenging whenever small time steps are required to resolve physics (e.g., transport-turbulence simulations) or computational (e.g., convergence issues for strongly nonlinearly coupled iterating modules) problems, or a high spatial resolution is needed for the selected plasma region or the modeling of the entire device. HLST supports the optimization of such first-principle codes; performs the parallelization of sequential codes using OpenMP and/or message passing interface (MPI) standards for massively parallel computers; improves the performance of existing parallel codes both at the single node and internode levels; assists the codes transfer to new multiprocessors architectures; and adapts/develops algorithms and/or mathematical library routines to improve applications for the targeted computer architectures. The codes recently supported by HLST in various physics areas are briefly described in Table I. These codes have been selected based on their potential contribution to the execution of the EUROfusion work program. As it is not possible to present the detailed improvements obtained for each code in a short overview, only the most significant HLST computational achievements helping to extend physics application domains of the first-principle codes are shown in Secs. III.A through III.D.

III.A. Core Physics: Transport, Turbulence, and Magnetic Reconnection

Self-consistent treatment of kinetic turbulence and magnetic reconnection is an example of a multiscale

TABLE I

Physics Codes Supported by HLST in 2015 and 2016

Area	Code	Physics Application	Plasma Model	HLST Support
Core physics: transport, turbulence, and magnetic reconnection	VIRIATO	From electron-scale turbulence and micro-tearing modes to magnetic reconnection and Alfvénic turbulence	Fluid-kinetic: asymptotically exact analytical reduction to 4D gyrokinetic ($\mathbf{r}$, $v_{\|\|}$) in low β_e limit	Modification of the parallel transpose algorithm for 2D FFT and assessment of its hybridization, I/O parallelization; 13 months support
	SFINCS	Neoclassical transport in nonaxisymmetric devices in 3D magnetic configuration, multiple plasma species	4D drift-kinetic equation for distribution function f, full-linearized FP collision operator	Code optimization, increase of robustness and efficiency; 6 months support
Edge, SOL and divertor physics	BIT2/BIT3	SOL: plasma, impurity, neutrals, PFC: particle and heat loads, PFC erosion, impurity generation	2D and 3D electrostatic PIC + direct MC code, Vlasov-Poisson equations	Development of 2D and 3D Poisson solvers, implementation of the MG technique; 6 months support
	BOUT++	SOL, divertor: turbulence and coherent structure motions in realistic geometry, edge-localized modes	Modular framework: reduced MHD or gyro-fluid type of equations in 3D curvilinear coordinates	Implementation of MG techniques in the module calculating Laplace inversions; 12 months support
	GBS	Turbulence dynamics in SOL: self-consistent evolution of fluctuations and plasma profiles	Drift-reduced Braginskii equations, Poisson equation, Ampere's law, kinetic neutrals, 3D geometry	Parallel MG solver (OpenMP + MPI) → (MPI + OpenACC), GBS adaptation to hybrid architecture computers; 12 months support
	GK MHD	Grad-Shafranov equilibrium solver for global core-edge SOL-divertor drift-wave turbulence simulations	Axisymmetric equilibrium model derived consistently from the gyrokinetic theory	Extension of a Poisson solver based on Sadourny's method beyond the X-point, into the SOL; 2 months support
	GRILLIX	Turbulence in the edge and SOL of diverted magnetic fusion devices	Full-f drift-reduced Braginskii equations, field line map approach for simulations across the separatrix	Extension of geometric MG solver to complex boundary conditions, improvement of hybrid (MPI + OpenMP) parallelization efficiency; 6 months support
	KIPP	Kinetic effects of parallel plasma transport in SOL and divertor	Vlasov-FP equation for $f_e(v_{\|\|}, v_{\perp}, l_{\|\|})$	Optimized distribution of the input arrays for MUMPS; 6 months support
	SOLPS	SOL and divertor physics: particle and heat loads, transport of charged species, atomic processes	Multifluid charged species (Braginskii equations), kinetic neutrons (MC)	Hybrid SOLPS package: OpenMP parallelization of B2, coupling with MPI EIRENE; 15 months support

(Continued)

TABLE I (Continued)

Area	Code	Physics Application	Plasma Model	HLST Support
	TOKAM3X	SOL and divertor: 3D turbulence and transport simulations in realistic geometry	Drift-reduced Braginskii equations	Profiling of sequential and hybrid (MPI + OpenMP) code, communication optimization; 6 months support
MHD	JOREK -STARWALL	Edge MHD stability and edge-localized modes, resistive wall modes, vertical displacement events, and disruptions	Reduced and full MHD with extensions for two-fluid and neoclassical physics, as well as vacuum/resistive walls	MPI parallelization of STARWALL and the coupling terms in JOREK; 12 months support
Radio frequency propagation and absorption, plasma-wave interaction	COCHLEA	Wave propagation in wave-guide structure of any complexity	Full-wave model: Maxwell's equations solver for cylindrical geometries	Hybrid (MPI + OpenMP) parallelization of original partially OpenMP parallelized code; 3 months support
	FWTOR	RF wave propagation and absorption relevant to Electron Cyclotron (EC)/Ion Cyclotron (IC)/Lower Hybrid (LH)/ Heating and Current Drive (H&CD), mm-diagnostics, and MHD control	Full-wave model: Maxwell's equations, plasma response formulated in terms of the generated electric current	Hybrid (MPI + OpenMP) parallelization of sequential code, introduction of parallel I/O and restart functionality; 18 months support
	MAG PICP	Physics of RF plasma sheath: plasma interaction with material surfaces, erosion, impact on heating efficiency	PIC + direct (collisions between MC particles) and conventional (collisions with background) MC approach	MPI parallelization compatible with existing OpenMP instructions; 6 months support
	REFMULX/ REFMUL3	2D and 3D full-wave simulations of O- and X-mode reflectometry	Maxwell's equations, with plasma effects included via response of electron current density to the electric field of the probing wave	Optimization of the sequential code and hybrid MPI + OpenMP parallelization; 12 months support
	RFDINITY	ICRF wall conditioning and discharge initiation	PIC-MC model: electron motion along B_{tor}, accelerated by RF field and by the electric field (Poisson equation)	Optimal algorithm to include Coulomb collisions, optimization of the MPI parallel code; 5 months support

problem, computationally challenging for modern five-dimensional gyrokinetic codes. The dimension of the problem can be reduced to four dimensions [three-dimensional (3D) configuration space and velocity parallel to the magnetic field] in the low-electron β_e limit $\beta_e \sim m_e/m_i$, where m_e and m_i are the electron and ion mass, respectively, while retaining key physics such as phase mixing and electron Landau damping, ion finite Larmor radius effects, electron inertia, electron collisions, and ohmic resistivity. This approach has been implemented in VIRIATO (Ref. 7), a novel fluid-kinetic code which solves four-dimensional (4D) gyrokinetic equations in combination with a kinetic reduced magnetohydrodynamic (MHD) model derived by expanding the gyrokinetic equation in terms of the small parameter $k_\perp \rho_i \ll 1$ (long wavelength limit of gyrokinetics), with $k_\perp$ being the wave number and ρ_i the ion Larmor radius. With this approach, VIRIATO can be applied to strongly magnetized, weakly collisional plasma dynamics in slab geometry to study Alfvénic plasma turbulence and magnetic reconnection.

The original VIRIATO code is parallelized with MPI using domain decomposition over two directions in the configuration space, one in the plane perpendicular to the magnetic field where a pseudo-spectral approach is used, and the other along the magnetic field, where a high-order upwind scheme is employed. With this parallelization involving the standard MPI algorithms, VIRIATO performance is close to the ideal strong scaling at small to medium numbers of cores (up to 2048 cores in the analyzed case). However, it strongly deviates from this scaling when a large number of cores is used, due to the negative effect of the network latency on the data transposition involved in the standard bi-dimensional (2D) fast Fourier transform (FFT). Within the activities of the HLST, the parallel scalability of VIRIATO has been improved by developing new efficient transpose algorithms for the 2D FFT (Ref. 8). The main idea of these algorithms is the data aggregation before carrying the all-to-all communication patterns to avoid penalizations due to network latency accumulation. The execution time of the 2D FFT has been reduced by one order of magnitude with these algorithms as compared to the original algorithm. The deployment of the new algorithms in VIRIATO allows one to achieve speedup factors close to 3 with small numbers of cores and of about 1.5 with large numbers of cores (Fig. 2). While the former eases future developments of the code by making smaller test cases more affordable, the latter is of particular importance for physics studies. It is useful, for example, for the investigation of the dependencies and parameter space for new physics phenomena, such as electron heating caused by reconnection in strongly magnetized, weakly collisional plasmas, or the effect of Landau damping on the turbulence energy spectra.

HLST support has been provided to a new stellarator neoclassical code SFINCS that can be used for neoclassical transport studies in nonaxisymmetric magnetic configuration.[9] SFINCS solves the 4D drift-kinetic equation for the distribution function, retaining coupling in two spatial independent variables and two velocity independent variables. It allows for 3D magnetic configurations, multiple plasma species, and employs the full

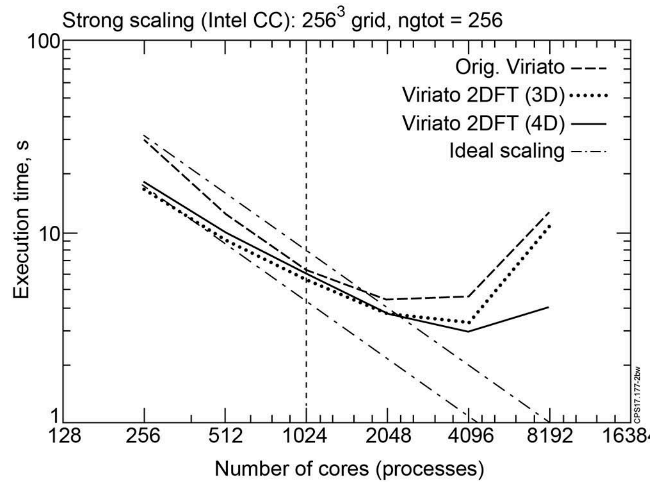

Fig. 2. Execution time of the VIRIATO code obtained with no data aggregation (dashed curve), 3D data aggregation (dotted curve), and 4D data aggregation (solid curve).

linearized Fokker-Planck (FP) collision operator with no expansion made in mass ratio. The code retains terms in the drift-kinetic equation which are often neglected in other numerical tools but can be important, e.g., when studying plasma impurities. A multifrontal massively parallel sparse direct solver (MUMPS) has been identified as the most time-consuming element of the SFINCS code and the performance of the alternative solvers implemented in SFINCS for testing (MKL-CPARDISO and HYPRE) has been investigated using 22 test cases.[10] All 22 tests were passed by MKL-CPARDISO with higher memory consumption (by 33% on average) than MUMPS, and 20 of these cases had better execution time with MUMPS (by 123% on average). None of the test cases was successfully terminated with HYPRE, possibly because HYPRE is more efficient for diagonal dominant problems while SFINCS is advection dominated, with small diagonal elements. Therefore, MKL-CPARDISO and HYPRE were discarded. Moreover, the performance of MUMPS within SFINCS has been further improved by optimizing its memory consumption.

III.B. Edge, SOL and Divertor Physics

Comprehensive and accurate modeling of scrape-off layer (SOL) and divertor plasma requires a self-consistent treatment of multiple charged species in real 2D or 3D geometry including their turbulence-driven as well as collisional transport, neutral and atomic physics, and plasma-wall interactions. This is an extremely challenging task for a single computational tool. Present codes are focused on advanced physics descriptions of some of these phenomena while using simplified approaches for others. Limiting this overview to the codes supported by HLST, the SOLPS package[11] is presently a main tool for understanding the plasma behavior in the SOL and divertor on existing European machines, including the effects of plasma transport and radiation, distribution of heat and particle loads on the divertor plates, poloidal asymmetries, and the role of drifts. SOLPS is based on 2D fluid Braginskii equations solved with ad-hoc transport coefficients for multiple charged species (B2 code[12]) combined with the Monte-Carlo (MC) technique for neutral simulations (EIRENE code[13]) in realistic 2D geometry. SOLPS modeling can be complemented with more detailed studies of kinetic effects of parallel plasma transport as included in KIPP (Ref. 14) and first-principle turbulence-transport simulations based on drift-reduced Braginskii equations solved under different assumptions for neutrals and magnetic topology [BOUT++ (Ref. 15), GBS (Ref. 16), GRILLIX (Ref. 17), and TOKAM3X (Ref. 18)]. Finally, the BIT family of codes[19] based on the PIC-MC technique represents an advanced first-principle approach where atomic physics, electrostatic turbulence [BIT2 (Ref. 20) and BIT3] and transport are treated self-consistently. The extended physics applications of the SOLPS package, one of the edge turbulence codes (GBS), and the BIT2-BIT3 codes which became available to users following the HLST code development work are described below.

Significant efforts were aimed at the OpenMP parallelization of B2. First, several B2 subroutines were optimized to reach a speedup close to the bandwidth limit leading to the reduction of the computation time of the sequential B2 version by 20% for the selected test case as compared to the original code. Second, more than 25 subroutines have been parallelized reaching 90% of parallelism in the whole B2 code. With these changes, a factor 6 speedup has been achieved for the ITER test case when executed on a single compute node (Fig. 3a). (Ref. 21). The improvement of EIRENE was further required to get an advantage from the parallelized B2 code in the coupled B2-EIRENE system. A simple and balanced parallelization strategy (all MPI processes calculate all strata and distribute particles evenly between the processes) was implemented in the ITER version of EIRENE to avoid a load imbalance when a limited number of cores (up to 16 cores) is used leading to an important speedup of the simulations (Fig. 3b). The coupled OpenMP B2 and the improved EIRENE codes will be of particular interest for time-consuming studies with SOLPS, such as parameter scans aimed to the optimization of the operational scenarios toward a detached divertor.

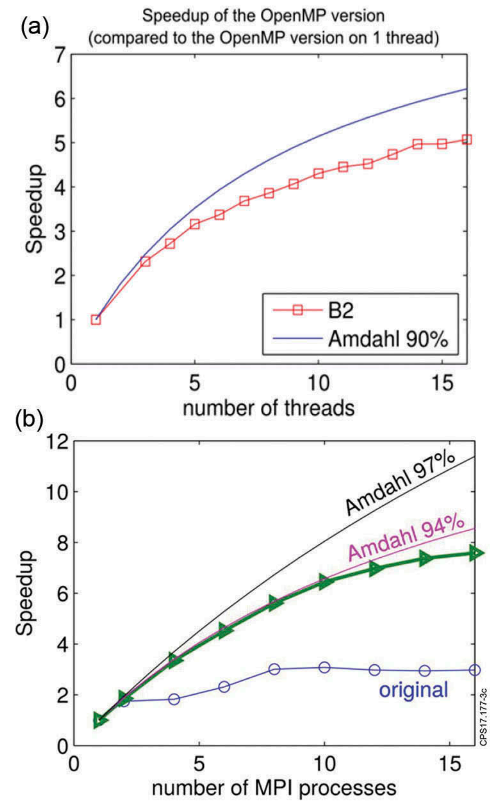

Fig. 3. (a) The speedup of B2 for ITER test case and (b) speedup of EIRENE for the AUG test case (solid curve with triangles). The Amdahl (ideal) scaling corresponding to the indicated parallel fraction of the code is shown for comparison.

Within HLST activities, a parallel multigrid (MG) solver has been developed for the GBS code using finite differences. With this solver, GBS is now capable to run both the simple electrostatic and more sophisticated electromagnetic simulations with respective gain factors of 5 and 10 compared to using the MUMPS direct solver. One important application for the improved GBS is the investigation of SOL turbulence self-consistently with the neutral dynamics implemented recently in this code.[22]

Presently, the BIT2 code simulates multiple plasma species and neutrals in the 2D space using ad-hoc anomalous cross-field diffusion coefficients. Although it is capable to simulate electrostatic turbulence self-consistently with plasma profiles, these simulations would be extremely time consuming taking into account the typically small simulation time step ($\approx 10^{-12}$ s) needed to resolve the Debye shielding and Larmor rotation, while the characteristic SOL turbulence time is much larger (10^{-4} to 10^{-5} s) and its accounting requires long simulations. A 2D MG solver was developed and implemented in BIT2 and a 3D MG solver with finite difference and finite element methods was also developed to solve larger problems on large numbers of MPI tasks in a reasonable timescale.[23] With this improvement, the BIT2 and BIT3 codes can be used for realistic fully kinetic simulation of the tokamak SOL and divertor plasma as well as for the linear plasma devices to more accurately predict the plasma behavior in SOL, particle, and energy loads to the plasma-facing components (PFCs), PFC erosion, and impurity and dust generation.

III.C. Radio Frequency Wave Propagation and Absorption, Plasma-Wave Interaction

Asymptotic methods for solving the wave equation in the short-wavelength limit (e.g., ray and beam tracing) are generally computationally fast and give sufficiently accurate calculations of the heating power needed, for example, for transport studies. However, problems like mode conversion, wave dispersion due to density fluctuations, prediction of high spatial resolution (few millimetres) diagnostics or neoclassical tearing mode stabilization by driving a well-localized radio frequency (RF) current require a computationally demanding full-wave modeling. HLST efforts have been devoted to three full-wave codes including REFMULX (Refs. 24 and 25), FWTOR (Refs. 26 and 27), and COCHLEA (Refs. 27 and 28), which have different physics applications (Table I). These codes solve the Maxwell's equations using a finite-difference time-domain numerical technique, which requires a fine spatial grid discretization to minimize the error and a high-resolution time discretization to comply with the conditions for convergence. Also, as the size requirements increase in an effort to simulate large devices, memory demands become important.

Remarkable results have been achieved in the speedup of the 2D REFMULX code due to the optimization of its sequential version with subsequent hybrid (OpenMP + MPI) parallelization (speedup factor over 400 on 512 cores as compared to the original sequential code) (Fig. 4) (Ref. 25). The ongoing parallelization of the 3D version of this code (REFMUL3), based on the experience gained with the 2D version, will augment the capabilities of reflectometry simulation enabling the modeling of ASDEX Upgrade or JET experiments much more accurately and predicting with more reliability the behavior of reflectometry in ITER or DEMO. REFMUL3 can also be a useful computational tool for interpretation of phenomena involving polarization changes, such as mode conversion and cross-polarization scattering by plasma fluctuations. The physics problems which can be investigated following

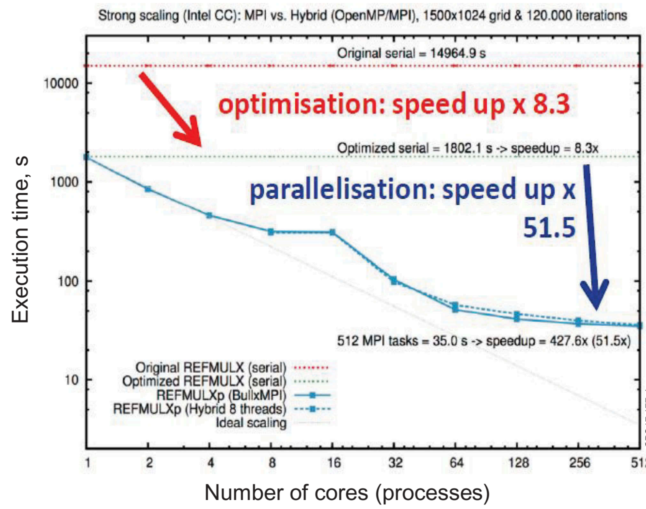

Fig. 4. Execution time obtained with the original REFMULX code (red dotted-dashed line), its optimized version (blue dotted line), and MPI parallel versions (blue solid and dashed curves).

HLST support to other codes include a wave propagation in complex geometries, such as the gyrotron beam tunnel (COCHLEA), O-X-B mode conversion, wave-driven parametric instabilities and high-resolution wave-based diagnostic measurements (FWTOR), the effect of magnetic field angle on sheath behavior in realistic experimental conditions (MAGPICP), and ion cyclotron resonance frequency (ICRF) breakdown conditions [RFDINITY (Ref. 29), see also Ref. 30 describing the optimization of this code].

III.D. Magnetohydrodynamics

Large-scale plasma instabilities affected by currents in conducting vessel structures can be modeled by solving the MHD equations in realistic toroidal X-point geometry coupled to a model for vacuum region and resistive conducting structures. This can be done with the coupled JOREK-STARWALL codes,[31] which are currently being extended to include the halo currents in collaboration with the ITER Organization. Although JOREK (Ref. 32) is MPI + OpenMP parallelized and STARWALL (Ref. 33) is partially OpenMP parallel, the coupled codes did not allow resolving realistic wall structures with a large number of wall elements (triangles) due to the consumption of wall clock time and memory. With HLST support the STARWALL code has been efficiently MPI parallelized enabling faster production runs (Fig. 5) (Ref. 34) or alternatively allowing simulations with much larger numbers of finite elements within a given time as

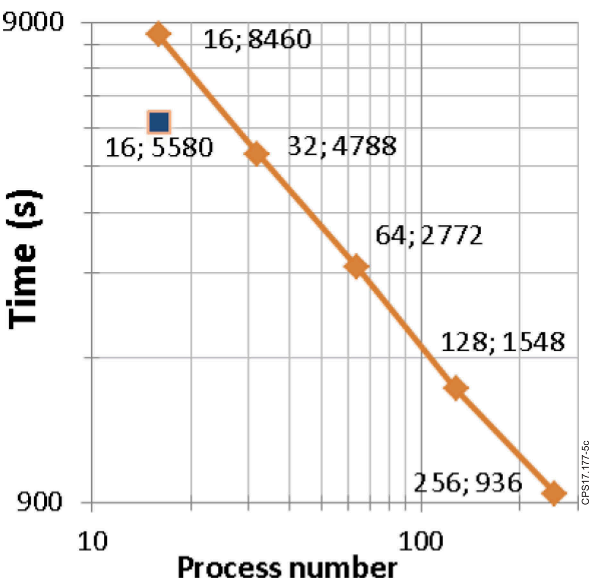

Fig. 5. Scaling of the total wall clock time in the MPI parallel STARWALL code (solid curve with squares). The numbers next to the symbols indicate the number of processes and computation time. The standalone single square corresponds to the original code (16 OpenMP threads).[34]

compared to the original code. Such improvement is particularly important for ITER simulations where the accounting of precise current patterns is required for the prediction of asymmetric forces acting on support structures during disruption events.

III.E. Development of Multicode Applications and General User Support

Modern parallel codes that address the physics issues mentioned above are becoming more and more sophisticated. They are composed of a growing set of submodels, including complex numerical and parallelization schemes, and accept an increasing number of input parameters. Tests are to be devised to detect bugs, cross-check the parallel algorithms and numerical schemes against available verification procedures, and check the parallel performance of these codes. These tests should be automated and triggered either each time the code repository is modified or periodically. With this purpose in mind, the Non-Regression Testing Suite (NRTS), including a minimal set of unit and regression tests, was developed by the Institute for Magnetic Fusion Research/CEA in collaboration with Maison de la Simulation/CEA and the Institute for Development and Resources in Computer Science/CEA computing facility for GYSELA (Ref. 35), taking this code as an example. With HLST support, NRTS was ported from Jenkins on the Poincare HPC to Buildbot on the HELIOS HPC to make it available to HELIOS's GYSELA users.[36] The deployment strategy (launching the automated tests when required and performance tests—small strong/weak scaling tests—to monitor/report the execution time) was defined and implemented.[36] Future developments will include an extension of NRTS to other codes.

In addition to the code optimization, HLST provides support to European scientists running their codes on HELIOS at the International Fusion Energy Research Centre—Computational Simulation Centre (Japan), such as porting the codes and their adaptation to new architectures (e.g., Many Integrated Core or Graphic Processing Unit), and the analysis of the performance of the most advanced hardware by means of different microbenchmark tests. This support activity is extended to the HELIOS successor MARCONI-FUSION (Sec. II).

IV. TOWARD A NUMERICAL TOKAMAK: SUPPORT TO THE DEVELOPMENT OF IM TOOLS

The integration of the most advanced EU codes into a single IM tool would enable physicists to predict the full discharge evolution more accurately, taking into account a strong coupling between different physics processes (e.g., thermal and particle transport depends strongly on current profiles evolution and fast-ion behavior, core and SOL plasmas are strongly coupled in the presence of tungsten impurities, plasma control algorithms impose additional coupling of actuators with plasma parameters, etc.). The status of the development of this tool and recent physics applications are described in Ref. 37, while a short summary of the CPT technical achievements in support of this tool is given here. The CPT is in charge of the development and maintenance of the framework for the IM tool based on a generic data structure consisting of standardized physics-oriented I/O units, CPOs (Ref. 38), a multilanguage interface used for exchange of CPOs between IM codes (UAL) (Ref. 39), an automated physics actor generator for KEPLER software presently used as a graphical WF engine for the IM tool, and other infrastructure functionalities. Such an infrastructure is by essence completely generic and can treat any problem which can be described by the data model, in contrast to integrated transport codes[40–42] which are typically focused on solving a specific physics problem (mainly, solving time-dependent core transport equations coupled to a variety of sources and transport components). Recently, the performance of the complex

IM WFs was optimized by developing a generic coupling method between a multiphysics WF engine and an optimization framework.[43] The coupling architecture, using a socket-based communication library for exchanging data between the two frameworks, was developed in order to preserve their integrity. This enables optimization studies of a physical problem described as an IM WF, demonstrated with the optimization of a fusion reactor design, making use of genetic algorithms. The whole scheme has been parallelized and used with up to 256 CPUs.

Owing to the large number of physical components involved in sophisticated IM WFs, such as the European Transport Solver,[37] a rigorous WF release procedure has been recently developed. All WF components are tagged in a specific way under software versioning and then automatically integrated into the KEPLER WF engine as a given self-consistent version of the released physical software.

Following the progress in the development of the IM tools and the start of their installation in EUROfusion experiments, the CPT extended its activities beyond the technical support to the developers of the IM tool to include support to users applying the released IM WFs on physics issues.

The EU IM infrastructure described above has been used as a prototype for the development of the ITER Integrated Modelling and Analysis Suite (IMAS) infrastructure.[44,45] The key new feature in IMAS is a more flexible data model (the ITER physics data model) allowing the description of multiple time bases within a given interface data structure (IDS), thus enabling direct representation of experimental data. Moreover, the GIT-based version control of the IMAS infrastructure and physical components allows an easier local deployment of the whole infrastructure on various computers. CPT activities have been recently geared toward an increased cooperation with the ITER Organization on IMAS including the installation of IMAS in EUROfusion experiments, its upgrade with the tools used for data analysis within EUROfusion, and development of the conversion tools from CPO to IDS in a short term, as well as direct transition to code integration under IMAS. In this frame, the Access Layer has been connected to the Identity and Access Management (IDAM) tool to enable on-the-fly access to remote databases from local experiments which are not natively using the ITER physics data model. The mapping between the native experiment data model and the ITER physics data model is described via an experiment-specific plug-in connected to the IDAM client-server architecture. This opens a way to retrieve data from various fusion experiments in a unique, standardized format, namely the ITER physics data model. This tool is being tested on WEST, JET, and MAST experiments.

V. SUMMARY

Within EUROfusion code development and IM efforts, recent achievements through its HLST and CPT in support to multiscale theory-based simulations in various physics areas created a basis for the extension of the application domain of first-principle codes and enabled time-consuming parameter scans as well as application of the optimized computational tools to large devices like ITER and DEMO. This was not possible previously due to unreasonably large computational time demands. The code optimization and speedup have led to a more efficient use of the HPC resources by increasing the number of running codes and physics problems addressed. The support to the IM infrastructure via its further optimization based on the most recent achievements of computer science is efficiently provided by CPT. These EUROfusion teams are working in close collaboration with ITER-CT, making their most recent developments available to the ITER Organization (e.g., SOLPS development, IMAS upgrade with new functionalities). The new EUROfusion supercomputer MARCONI-FUSION and the Gateway started their operation hosting IM and HPC projects addressing the most challenging issues of fusion physics, materials modeling, and technology for existing machines, JT60-SA, ITER, and DEMO.

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