Recent EUROfusion achievements in support to computationally demanding multi-scale fusion physics simulations and integrated modelling

I. Voitsekhovitch[1,2], R. Hatzky[3], D. Coster[3], F. Imbeaux[4], D. C. McDonald[2], T. B. Fehér[3], K. S. Kang[3], H. Leggate[5], M. Martone[3], S. Mochalskyy[3], X. Sáez[6], T. Ribeiro[3], T.-M. Tran[7], A. Gutierrez-Milla[6], S. Heuraux[8], M. Hölzl[3], S. D. Pinches[9], F. da Silva[10], D. Tskhakaya[11], T. Aniel[4], D. Figat[12], L. Fleury[4], O. Hoenen[3], J. Hollocombe[2], D. Kaljun[13], G. Manduchi[14], M. Owsiak[12], V. Pais[15], B. Palak[12], M. Plociennik[12], J. Signoret[4], C. Vouland[4], D. Yadykin[16]

[1]*EUROfusion Programme Management Unit, Garching, Germany*
[2]*CCFE, UK Atomic Energy Authority, Culham Science Centre, Abingdon, OX14 3DB, UK*
[3]*Max-Planck-Institut für Plasmaphysik, Garching D-85748, Germany*
[4]*CEA, IRFM, F-13108 Saint-Paul-lez-Durance, France*
[5]*Dublin City University, Dublin, Ireland*
[6]*Barcelona Supercomputing Centre, 08034 Barcelona, Spain*
[7]*SPC-EPFL, 1015 Lausanne, Switzerland*
[8]*Institute Jean Lamour UMR 7198 CNRS-Université Henri Poincaré BP 70239 F-54506, Vandoeuvre, France*
[9]*ITER Organization, Route de Vinon-sur-Verdon, CS 90 046, 13067 St Paul Lez Durance Cedex, France*
[10]*Instituto de Plasmas e Fusão Nuclear- Laboratório Associado, 1046-001 Lisboa, Portugal*
[11]*Institute of Applied Physics, Vienna University of Technology, Fusion@ÖAW, A-1040 Vienna, Austria*
[12]*PSNC, Poznan Supercomputing and Networking Center, Poznan, Poland*
[13]*University of Ljubljana, Kongresni trg 12 · 1000, Ljubljana Slovenia*
[14]*Consorzio RFX, Corso Stati Unit 4, 35127 Padova, Italy*
[15]*National Institute for Laser, Plasma and Radiation Physics, PO Box MG-36, 077125 Magurele, Bucharest, Romania*
[16]*Chalmers University of Technology, S-41296 Göteborg, Sweden*

Abstract

Integrated Modelling (IM) of present experiments and future tokamak-reactor requires numerical tools which could simulate spatially multi-scale phenomena as well as dynamically fast transient events and relatively slow plasma evolution within a reasonably fast computational time. The progress in the optimisation and speedup of the EU first-principle codes and in the development of a basis for their integration into a centrally maintained suite of IM tools achieved by the EUROfusion High Level Support Team (HLST) and Core Programming Team (CPT) is presented. Physics phenomena which can be addressed in various areas (core turbulence and magnetic reconnection, edge and SOL physics, RF heating and current drive, MHD, reflectometry simulations) following code optimisation and parallelisation performed by HLST are briefly described. The CPT development activities in support to IM including a support to local deployment of the IM infrastructure and experimental data access, to the management of releases for sophisticated IM workflows involving a large number of components and to the performance optimization of complex IM workflows are briefly summarised.

1. Introduction

Mathematical modelling of strongly non-linearly coupled physics processes in magnetically confined fusion plasmas requires (i) the advanced first-principle physics codes capable to describe multi-scale phenomena within a reasonably fast computational time; (ii) integration of these codes into the unique Integrated Modelling (IM) suite; and (iii) large High Performance Computer (HPC) resources. The progress in the optimisation and speedup of the EU theory-based codes to adapt them to modern HPC architecture and in the development of a basis for integration of these codes into a centrally maintained suite of IM tools achieved by the EUROfusion High Level Support Team (HLST) [1] and Core Programming Team (CPT) in 2015–2016 is presented, with a particular emphasis on the physics phenomena which can be addressed following these developments.

2. Enabling efficient first-principle physics simulations

The progress in the development of fusion theory motivates further development of numerical tools capable to address new physics effects. Such effects are computationally challenging when a small time step is required to resolve the physics (e.g. transport-turbulence simulations) or computational (e.g. convergence issues for strongly non-linearly coupled iterating modules) problems, or a good spatial resolution is needed for the selected plasma region or the whole-device modelling. HLST supports the optimisation of such first-principle codes, performs parallelisation of sequential codes using OpenMP and/or MPI standards for massively parallel computers, improves the performance of existing parallel codes both at the single node and inter node 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 supported by HLST in 2015–2016 in various physics areas are briefly described in table 1. The most significant computational achievements and extended physics applications of the first-principle codes following the HLST developments are illustrated below using a few examples.

a) core physics: turbulence and magnetic reconnection

Self-consistent treatment of kinetic turbulence and magnetic reconnection is an example of the multi-scale problem, computationally challenging for modern 5D gyrokinetic (GK) codes. The problem dimension can be reduced to 4D (3D configuration space and velocity parallel to the magnetic field) in the low electron β_e limit ($\beta_e \sim m_e/m_i$) 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 [2], a novel fluid-kinetic code which solves 4D GK equations in combination with a kinetic reduced MHD model, derived by expanding the GK equation in terms of the small parameter $k_\perp \rho_i << 1$ (long wavelength limit of gyrokinetics). With this approach, VIRIATO can be applied to strongly magnetised, 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 parallelisation 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 analysed 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 fast Fourier transform (2D FFT). The parallel scalability of VIRIATO has been improved by developing new efficient transpose algorithms for the 2D FFT [3]. 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 three with small numbers of cores and of about 1.5 with large numbers of cores (Fig. 1). 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 the electron heating caused by reconnection in strongly magnetized, weakly collisional plasmas, or the effect of Landau damping on the turbulence energy spectra.

HLST support to the development of plasma core modelling tools is extended recently to include the SFINCS code [4] which is used for neoclassical transport studies in non-axisymmetric magnetic configurations.

b) edge, SOL and divertor physics

Comprehensive and accurate modelling of SOL and divertor plasma requires a self-consistent treatment of multiple charged species in real 2D or 3D geometry including their turbulence-driven and 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 the advanced physics description of some of these phenomena while using the simplified approaches to others. Limiting this overview to the codes supported by HLST, the SOLPS package [5] is presently a main tool for understanding the plasma behaviour in SOL and divertor on existing machines including the effects of plasma transport and radiation, distribution of heat and particle loads on the divertor plates, poloidal asymmetries and role of drifts. SOLPS is based on the 2D fluid Braginskii equations solved with the ad-hoc transport coefficients for multiple charged species (B2 code) combined with the Monte-Carlo (MC) technique for neutral simulations (EIRENE code) in realistic 2D geometry. SOLPS modelling can be complemented with the more detailed studies of kinetic effects of parallel plasma transport as included in KIPP [6] and the first-principle turbulence-transport simulations based on the drift-reduced Braginskii equations solved under different assumptions for neutrals and magnetic topology (BOUT++ [7], GBS [8], GRILLIX [9] and TOKAM3X [10]). Finally, the BIT family of codes [11] based on the PIC MC technique represents an advanced first-principle approach where the atomic physics, electrostatic turbulence (BIT2 and BIT3) and transport are treated self-consistently. The extended capabilities of the SOLPS package, one of the edge turbulence codes (GBS) and the BIT2-BIT3 codes following HLST support are described below.

Significant efforts were aimed at the OpenMP parallelisation 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 six speedup has been achieved for the ITER test case when executed on a single compute node (Fig. 2, top panel) [12]. The improvement of EIRENE was further required to get an advantage from the parallel 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. 2, bottom panel). Coupled OpenMP B2 and improved EIRENE codes will be of particular interest for the time-consuming studies with SOLPS, such as the parameter scans aimed to the optimisation of the operational scenarios towards a detached divertor.

With HLST support, 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 a respective gain of factors 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 [13].

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 the 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} – 10^{-5} s) and its accounting requires long simulations. The 2D MG solver was developed and implemented in BIT2 and the 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 time scale [14]. 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 the linear plasma devices to predict more accurately the plasma behaviour in SOL, particle and energy loads to the plasma facing components (PFC), PFC erosion and impurity and dust generation.

c) RF propagation and absorption, plasma-waves 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, such problems like mode conversion, wave dispersion due to density fluctuations, prediction of high-resolution mm-diagnostics or NTM stabilisation by driving a well-localised RF current require a computationally-demanding full-wave modelling. HLST support has been provided to three full-wave codes including REFMULX [15, 16], FWTOR [17, 18] and COCHLEA [19, 18], which have different physics applications (table 1). These codes solve the Maxwell's equations using a finite-difference time-domain numerical technique, which requires a fine spatial grid discretization to minimise 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 optimisation of its sequential version, with subsequent hybrid (OpenMP + MPI) parallelisation (the speedup factor over 400 on 512 cores as compared to the original sequential code, Fig. 3) [16]. The on-going parallelisation 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 modelling of ASDEX Upgrade or JET experiments much more accurately and predicting with more reality the behaviour 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 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), effect of magnetic field angle on sheath behaviour in realistic experimental conditions (MAGPICP) and ICRH breakdown conditions (RFDINITY [20], see also Ref. 21 describing the optimization of this code).

d) MHD

Large scale plasma instabilities affected by currents in conducting vessel structures can be modelled 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 [22], which are currently being extended to include the halo currents in collaboration with ITER Organization.Although JOREK is MPI+OpenMP parallelised and STARWALL is partially OpenMP parallel, the coupled codes did not allow to resolve the 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. 4) [23] or alternatively allowing simulations with much larger numbers of finite elements within a given time as 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.

e) development of multi-code 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 sub-models, include complex numerical and parallelization schemes and accept an increasing number of input parameters. Tests should 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 IRFM/CEA in collaboration with Maison de la Simulation/CEA and IDRIS computing facility for GYSELA [24] taking this code as an example. With HLST support NRTS was ported from Jenkins on Poincare to Buildbot on HELIOS to make it available to HELIOS' GYSELA users [25]. 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 [25]. Future developments will include an extension of NRTS to other codes.
In addition to the code optimisation, HLST provides support to European scientists running their codes on HELIOS at IFERC-CSC (Japan), such as porting the codes and their adaptation to new architectures (e.g. MIC or GPU), and analysis of the performance of the most advanced hardware by means of different micro-benchmark tests. This support activity is extended to the HELIOS successor MARCONI-FUSION (section 4).

3. Towards numerical tokamak: support to the development of IM tool

An 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 behaviour, core and SOL plasmas are strongly coupled in 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. 26, while a short summary of the CPT technical achievements in support to this tool is given here. The CPT is in charge for the development and maintenance of the framework for the IM tool based on a generic data structure consisting of standardised physics-oriented input/output units, called Consistent Physical Objects (CPOs), [27], the multi-language interface used for exchange of CPOs between IM codes (Universal Access Layer (UAL)) [28], the automated physics actor generator for KEPLER software, presently used as a graphical workflow engine for the IM tool, and other infrastructure functionalities. Recently, the performance of the complex IM workflows (WF) was optimised by developing a generic coupling method between a multi-physics WF engine and an optimization framework [29]. 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 [26], a rigorous WF release procedure has been recently developed. All WF components are tagged in a specific way under SVN, then automatically integrated to 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 the 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 developments of the ITER Integrated Modelling and Analysis Suite (IMAS) infrastructure [30, 31]. 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. The CPT activities have been recently geared towards an increased cooperation with ITER Organization on IMAS including the installation of IMAS in EUROfusion experiments, its upgrade with the tools used for the data analysis within EUROfusion, development of the conversion tools from CPO to ITER Data Structure (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 IDAM 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, standardised format, namely the ITER physics data model. This tool is being tested on WEST and MAST experiments.

4. Extension of EUROfusion computational capabilities (HPC MARCONI-FUSION)

The shutdown of the HELIOS supercomputer at IFERC-CSC presently used by the EU fusion scientists will take place at the end of 2016. Following the increasing need in the first-principle simulations and integrated modelling, a growing number of HPC users and success in code optimisation and speedup, the EU extended its technical computational capabilities by establishing a new HPC for Fusion Applications under EUROfusion. The first phase of the conventional partition (Intel Xeon-Broadwell processors, 1 Pflops) of this machine called MARCONI-FUSION is already operational and it will be replaced by the 5 Pflops Intel Xeon-Skylake processors by the third quarter of 2017. The accelerated partition will consist of 1 Pflops Intel Knights Landing (KNL) processors and will be upgraded to 50% GPU - 50% KNL in the fourth quarter of 2017. Part of the supercomputer resources is allocated to the Gateway hosting the IM tool developed by EUROfusion. Having the Gateway directly connected to HPC is an advantage for the users of the distributed WFs, i.e. the WFs executing partly on a distributed computer architecture of HPC and partly on the Gateway (for example, the WF for transport-turbulence simulations where the first-principle turbulence simulations can be done on HPC). For such WFs, the specific KEPLER actors for launching jobs on HPC and accessing CPO data remotely through the UAL [32], as well as a parallel-I/O extension of the UAL [33] were developed.

5. Summary

Recent HLST and CPT achievements in support to multi-scale theory-based simulations in various physics areas created a basis for an extension of the application domain of the first-principle codes and enabled time-consuming parameter scans as well as application of the optimised computational tools to large devices like ITER and DEMO. This was not possible previously due to unreasonably large computational time demands. The code optimisation and speedup leads to a more efficient use of the HPC resources by increasing the number of running codes and addressed physics problems. The support to the IM infrastructure via its further optimisation 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 Organisation (ex. SOLPS development, IMAS upgrade with new functionalities). The new supercomputer MARCONI-FUSION and the Gateway started their operation hosting the EUROfusion HPC projects addressing the most challenging issues of the fusion physics, materials and technology for existing machines, JT60-SA, ITER and DEMO.

Acknowledgment
This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014–2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

References
[1] R. Hatzky, *The experience of the High Level Support Team (HLST)*, 2nd IFERC-CSC Review Meeting, 17th March 2014, Rokkasho, Japan; see also http://www.efda-hlst.eu/;
[2] N. F. Loureiro *et al*, Phys. Rev. Lett. **111** 025002 (2013); see also http://arxiv.org/abs/1505.02649;
[3] T. Ribeiro, *Improving the scalability of the VIRIATO code*, IPP Theory Meeting, 23rd – 27th November 2015, Plau am See, Germany;
[4] M. Landreman *et al*, Phys. Plasmas **21** 042503 (2014);
[5] R. Schneider *et al*, Cont. Plasma Phys. **46** 3 (2006);
[6] A. V. Chankin *et al*, Cont. Plasma Phys. **52** (5-6) 500 (2012);
[7] B. D. Dudson *et al*, Comp. Phys. Comm. **180** 1467–1480 (2009);
[8] P. Ricci *et al*, Plasma Phys. and Contr. Fusion **54** 124047 (2012);
[9] A. Stegmeir *et al*, Comp. Phys. Comm. doi:10.106/j.cpc.2015.09.016 (2015);
[10] P. Tamain *et al*, Cont. Plasma Phys. **54** 555 (2014);
[11] D. Tskhakaya, Cont. Plasma Phys. **52** (5-6) 490 (2012);
[12] T. Fehér, *SOLPS Parallel Optimization*, SOLPS Opt. Working Session, 30th November 2015, IPP-Garching, Germany;
[13] C. Wersal and P. Ricci, Nucl. Fusion **55** 123014 (2015);
[14] K. S. Kang, Computational Methods in Applied Mathematics **15** 189 (2015);
[15] F. da Silva *et al*, J. Comp. Physics, 295: 24-45 (2015); F. da Silva *et al*, 42nd EPS Conference on Plasma Physics, P4.175, Lisbon, Portugal, 22nd - 26th June 2015;
[16] T. Ribeiro, F. da Silva, *Parallelization of the X-mode reflectometry full-wave code REFMULX*, 28th October 2014, IPP, Garching, Germany;
[17] C. Tsironis *et al*, Bull. Am. Phys. Soc., vol. **58**, art. 8.80 (2013)
[18] M. Martone, bi-annual HLST meetings 14th October 2015 and 19th April 2016, IPP Garching, Germany;
[19] D. V. Peponis *et al*, "FDTD simulation of a cylindrical waveguide using longitudinal current distribution as an excitation scheme", PIERS 2015: 6th -9th July 2015, Prague, Czech Republic
[20] M. Tripský *et al*, 41st EPS Conf. Control Fusion and Plasma Physics, Berlin, Germany, 23-27 June, 2014;
[21] H. Leggate, bi-annual HLST meeting, 13th October 2016, IPP Garching, Germany;
[22] M. Hölzl *et al*, JPCS **401** 012010 (2012);
[23] S. Mochalskyy *et al*, Report of the EUROfusion High Level Support Team Project JORSTAR 2016;
[24] V. Grandgirard *et al*, AIP Conf. Proceedings, **871**, 100-111 (2006);
[25] X. Sáez, bi-annual HLST meeting, 19th April 2016, IPP Garching, Germany;
[26] G. Falchetto *et al*, this conf.; see also G. L. Falchetto *et al*, Nucl. Fusion **54** 043018 (2014);
[27] F. Imbeaux *et al*, Comp. Phys. Comm. **181** 987 (2010);
[28] G. Manduchi *et al*, Fusion Eng. Design **83** 462 (2008);
[29] L. Di Gallo, C. Reux, F. Imbeaux *et al*, Comp. Phys. Comm. **200** 76 (2016);
[30] F. Imbeaux *et al*, Nucl. Fusion **55** 123006 (2015);
[31] S. Pinches *et al*, this conf.;
[32] P. I. Strand *et al*, Fusion Eng. Design **85** 383 (2010);
[33] A. Galonska *et al*, Comp. Phys. Comm. **184** 638 (2013)

Table 1. Physics codes supported by HLST in 2015-2016

Area	Code	Physics application	Plasma model	HLST support
Core physics	*VIRIATO*	From electron-scale turbulence (ETG, micro-tearing modes) to magnetic reconnection and Alfvénic turbulence	Fluid-kinetic: asymptotically exact analytical reduction to 4D GK (**r**, $v_{//}$) in low β_e limit	Modification of the parallel transpose algorithm for 2D FFT and assessment of its hybridisation, I/O parallelisation
	SFINCS	Neoclassical transport in non-axisymmetric devices in 3D magnetic configuration, multiple plasma species	4D drift-kinetic equation for f, full linearized FP collision operator	Increase robustness and efficiency by replacing the MUMPS library
Edge, SOL and divertor physics	*BIT2 / BIT3*	SOL (plasma, impurity, neutral transport), PFC: particle and heat loads, PFC erosion, impurity generation	2D-3D electrostatic PIC+ direct Monte Carlo (MC) code, Vlasov-Poisson eqs.	Development of 2D and 3D Poisson solvers, implementation of the Multi-Grid (MG) technique
	BOUT ++	SOL, divertor: turbulence and coherent structure motions in realistic geometry, ELMs	Modular framework: reduced MHD or gyro-fluid type of eqs in 3D curvilinear coordinates	Implementation of MG techniques in the module calculating Laplace inversions
	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
	GKM HD	Grad-Shafranov equilibrium solver for global core-edge-SOL-divertor drift-wave turbulence simulations	Axisymmetric equilibrium model derived consistently from the GK theory	Extension of a Poisson solver based on Sadourny's method beyond the X-point, into the SOL.
	GRILLIX	Turbulence in the edge and SOL of diverted magnetic fusion devices	Full-f drift-reduced Braginskii eqs, field line map approach for simulations across the separatrix	Extension of geometric MG solver to complex boundary conditions, improvement of hybrid (MPI+OpenMP) parallelisation efficiency
	KIPP	Kinetic effects of parallel plasma transport in SOL and divertor	Vlasov-Fokker-Planck equation for $f_e(v_{\|\|}, v_{\perp}, l_{\|\|})$	Optimised distribution of the input arrays for MUMPS
	SOLPS	SOL and divertor physics: particle and heat loads, transport of charged species, atomic processes	Multi-fluid charged species (Braginskii eqs), kinetic neutrons (MC)	Hybrid SOLPS package: OpenMP parallelization of B2, coupling with MPI EIRENE
	TOKA M3X	SOL and divertor: 3D turbulence and transport simulations in realistic geometry	Drift-reduced Braginskii equations	Profiling of sequential and hybrid (MPI+OpenMP) code, communication optimisation.
MHD	*JOREK - STARWALL*	Edge MHD stability and ELMs, RWMs, VDEs and disruptions.	Reduced MHD equations, model for the vacuum region and the resistive conducting structure.	MPI parallelization of STARWALL and the coupling terms in JOREK
RF propagation, plasma-wave interaction	*COCH LEA*	Wave propagation in wave-guide structure of any complexity	Full-wave model: Maxwell's equations solver for cylindrical geometries	Hybrid MPI+OpenMP parallelisation of original partially OpenMP parallelised code
	FWTOR	RF wave propagation & absorption relevant to EC/IC/LH H&CD, mm-diagnostics and MHD control	Full-wave model: Maxwell's equations, plasma response is formulated in terms of the generated electric current	Hybrid (MPI + OpenMP) parallelisation of sequential code, introduction of parallel I/O and restart functionality
	MAG PIC	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 parallelisation compatible with existing OpenMP instructions
	REFMULX / REFMUL3	2/3D 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	Optimisation of the sequential code and hybrid MPI-OpenMP parallelisation
	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, optimisation of the MPI parallel code

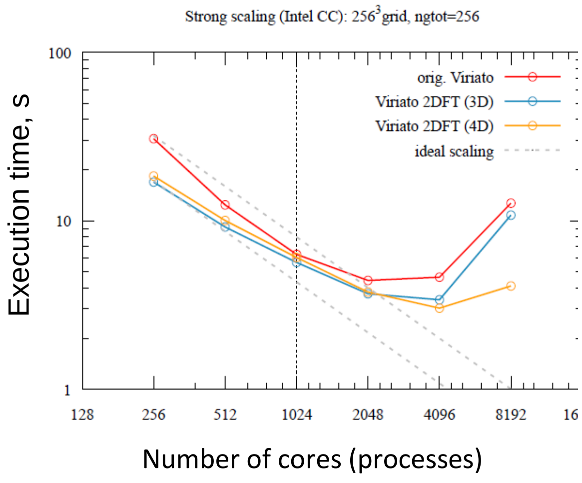

Fig. 1. Execution time of the VIRIATO code obtained with no data aggregation (red), 3D data aggregation (blue) and 4D data aggregation (yellow).

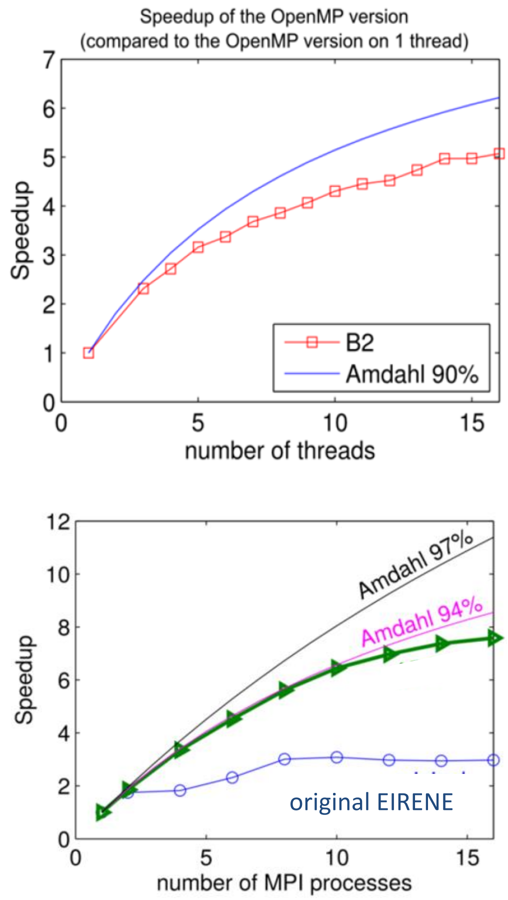

Fig. 2. Speedup of B2 for ITER test case (top) and speedup of EIRENE for the AUG test case (bottom, green symbols). The Amdahl (ideal) scaling corresponding to the indicated parallel fraction of the code is shown for comparison.

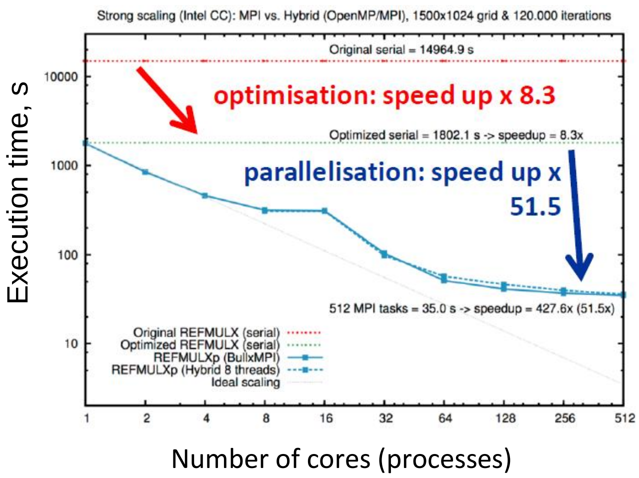

Fig. 3. Execution time obtained with the original REFMULX code (red dotted-dashed), its optimised version (blue dotted) and MPI parallel version (blue solid).

Fig. 4. Scaling of the total wall clock time in the MPI parallel STARWALL code (yellow squares). The numbers next to the symbols indicate the number of processes and computation time. The blue square corresponds to the original code (16 OpenMP threads) [21].