High Performance Computing under EURATOM-MEdC Programe

Iulian PETRISOR

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Overview

- HPC – G Steinbrecher (UCv)
- DATARoom (UCv)
- HPC – Iulian Petrisor (UCv)
- Teams/peoples/needs under EURATOM/EUROFusion Program
- few info about new EUROFusion …

Algorithm development for scientific computing

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Integrated Tokamak Modeling (ITM)

- The Integrated Tokamak Modeling Task Force coordinates the European Modeling activities under the European Fusion Development Agreement (EFDA). http://portal.efda-itm.eu/itm/portal/
- Provides the software infrastructure for the simulation of large thermonuclear fusion reactors with magnetic confinement, mainly tokamaks.

Integrated Tokamak Modeling

- Elaboration of improved orbit following Monte Carlo methods for Fokker –Planck equation that models the plasma heating in thermonuclear fusion reactors with magnetic confinement. The studies were performed in the framework of the project Integrated Tokamak Modelling, http://portal.efda-itm.eu/itm/portal/
- New class of stochastic integrators of singular stochastic differential equation with singularities: G. Steinbrecher, R. J. Dumont "Numerical Instabilities in the Accelerated Orbit Following Monte-Carlo Method", ITM General Meeting 2010, Lisbon.
- Acces to Gateway, Rechenzentrum Garching, Max Planck Institute for Plasma Physics (http://www.rzg.mpg.de/)

ITM: New stochastic methods for the Fokker-Planck equation

- Foundation of new numerical algorithm for simulation of instability growth in turbulent plasma in tokamak
- Steinbrecher G., Weyssow B., Phys. Rev. Lett. 92, 125003 (2004).
- G. Steinbrecher, X. Garbet, B. Weyssow, "*Large time behaviour in random multiplicative processes*", arXiv:1007.0952v1 [math.PR], (2010).

ITM: New Mont-Carlo methods for Fokker-Planck equation

- R. Dumont, T. Mathurin, M. Schneider, L.-G. Eriksson, T. Johnson and G. Steinbrecher. *Advanced simulation of energetic ion populations in the presence of NBI and RF sources*, The 12th Meeting of the ITPA Energetic Particle, Topical Group. March 31-April 3, 2014, CIEMAT, Spain
- http://fusionsites.ciemat.es/itpaep2014/files/2014/03/AgendaITPA12.pdf

ITM: New methods for solution of the stationary Fokker-Planck equations

- Numerical approximations obtained from the principle of maximal entropy and minimal entropy production :
- Sonnino G., Steinbrecher G., Cardinali A., Sonnino A., Tlidi M. *Family of probability distributions derived from maximal entropy principle with scale invariant restrictions.*, Phys. Rev. **E 87**, (2013), 014104-1, 014104-5.
- Sonnino G., Cardinali A., Steinbrecher G., Peeters P., Sonnino A., Nardone P., *Reference Distribution Functions for Magnetically Confined Plasmas from the Minimum Entropy Production Theorem and the MaxEnt Principle, subject to the Scale-Invariant Restrictions*, Physics Letters **A 377**, (2013) 3061-3077.
- Sonnino G., Steinbrecher G., *Generalized class of reference distribution functions for use in gyrokinetic simulations*. Accepted to Romanian Reports in Physics 2014.

Signal Processing

- Numerical treatment of the classical Hausdorff Moment Problem, with application in RMN: . G. Steinbrecher, R. Scorei, V. Cimpoiasu, I. Petrisor *"Stable Reconstruction of the T2 Distribution by Low Resolution NMR Measurement and the Classical Markov and Hausdorff Moment Problem"*. Journal of Magnetic Resonance, **146**, 321-334 (2000).
- Causality detection in random signals, entropy methods: Sonnino G., Steinbrecher G., *New Class of Generalized Extensive Entropies for Studying Dynamical Systems in Highly Anisotropic Phase Space*, arXiv:1311.4790v1 [cond-mat.stat-mech] (2013) Phys. Rev. **E 89**, 062106 (2014)

Generation of fractional super diffusive Brownian motion

- Fractional Brownian motion was introduced by A. N. Kolmogorov for modelling developed turbulence.
- Numerical algorithm: G. Steinbrecher, B. Weyssow "*New representation and generation algorithm for fractional Brownian motion*", Romanian Journal of Physics, 55,1120-1130, (2010).
- The algorithm uses: Steinbrecher G., Weyssow B., Physical Review Letters 92, 125003 (2004).

Numerical methods for quantile of some classical probability distributions

- Series representation for the quantile of normal, student, gamma, beta probability distributions : G. Steinbrecher, W. T. Shaw. *"Quantile Mechanics"*, European Journal of Applied Mathematics, 19, 87, (2008).
- The representation for normal distribution quantile: http://functions.wolfram.com/GammaBetaErf/InverseErf/06/01/02/0004/

DataRoom

General Presentation

University of Craiova
Faculty of Mathematics and Natural Sciences
Research Lab: MANA
Contact: nikyc@central.ucv.ro

Computing power:

1. High speed interconnection network managed centrally able to increase the interoperability with other research centers;
2. Over 350 GB RAM;
3. Computing power capable of supporting a large amount of virtual machines available remotely, managed with VMware VSphere, optimized solution for cloud computing;
4. Redundant storage of over 20 TB.

Infrastructure:

- All equipment within the DataRoom are redundant, so in case of technical problems, all systems are functional;
- Network Core 10 GBe interconnects, at the same speed. All rooms where the core provides data traffic at CAT6 standard with Fiber Optic;
- Firewall Server that protects the network of the entire system.

Usage:

- With the DataRoom we can provide virtual machines with high power for complex mathematical computation;
- High performance computing power that ensures data availability at all times so that all vital functions operating data from the research laboratories can maintain activity;

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Review of previously studies that involved HPC...

In cadrul unor directii de lucru ale grupului EURATOM – MEdC, de la Universitatea din Craiova (UCv) Romania, s-au utilizat sistematic, incepind cu 2004, diverse facilitati de calcul (puse la dispozitie in cadrul contractelor de colaborare), prin urmatoarele computere paralele:

- ***IXIA si Chrome– two projects:CEA Cadarache (France), ULB (Belgium) and UCv (Romania) (2003-2005)***
- ***ANIC and ASTER (paralell computers of ULB/VUB, 2003-2009)***
- ***Cobra and Viper, Hydra (ULB facilities, 2010 → ...)***

Mainly, the research studies, with contributions to Integrated Tokamak Modelling Task Force (EFDA ITM-TF) and EFDA MHD, involved:

- The diffusion of magnetic field lines in tokamaks, in various stochastic fields
- The diffusion of charged particles in tokamaks, in various stochastic fields
- Zonal flow generation in tokamaks (Zonal Flow structures)

Review of previously studies that involved HPC...

Under EFDA MHD we developed (***PTRANSP***) – *HPC-FF project (2010-2012)*

- **Project Title** - ***Test particle transport in turbulent magnetohydrodynamics***
- **Project Acronym** - *PTRANSP*

Team: Daniele Carati (ULB), C. Lalescu (ULB and UCv), M. Negrea (UCv), I. Petrisor (UCv).

- **Types of Requirements**
- Computer resource requirements: Total amount of CPU hours: 385000 + 800 000
- Computer resource requirements:
  Average and maximum number of CPUs per job: average 64/maximum 128

Charged particle transport in a turbulent plasma is influenced by large scale structures as well as by small scale fluctuations of the electromagnetic field. Specific scenarios of magnetohydrodynamic (MHD) flows with large scale structures are studied at different degrees of turbulence, and trajectories for several species of passive particles (in these flows) were computed.

Review of previously studies that involved HPC...

Proposal for an IFERC-CSC Project

(for the **Project cycle 2** from 15th November 2012 to 14th November 2013)

- **Project Title** - ***Influence of small-scale structures on test-particle transport in turbulent plasmas***
- **Project Acronym** - *S3TP2*

Team: Bernard Knaepen *(ULB)*, Lapo Bettarini*(ULB)*, *M. Negrea (UCv)*, *I. Petrisor (UCv)*.

- **Types of Requirements**
- Computer resource requirements: Total amount of CPU hours: + 800 000

...The purpose of our proposal is to study test-particle transport and acceleration in magnetic fields obtained by highly accurate numerical simulations of magneto-hydrodynamics (MHD) systems. Our aim is: to relate the particle diffusion-coefficient properties to the characteristics of the electromagnetic fields; to study the influence of small-scale structures on particle transport and to mimic their role in more and more realistic closed models..

Review of previously studies that involved HPC...

Total amount of requested node hours for the present project (one node corresponds to 16 cores)	100000
Expected average and maximum number of nodes per run	Avg: 8, Max: 16
Expected minimum number of nodes per run based on memory requirements [note that up to 58 GB per node (= 16 cores) are available]	4
Temporary disk space required for a single run [for input / output / restart files etc.]	500 Gb
Permanent disk space required for the entire project [if larger than 10 TB]	10 Tb
Retention time of the obtained data	2 months
Estimated volumes of data transferred to/from IFERC-CSC by network	To: ~ almost zero From: 10T
Use of visualization cluster?	Yes
Name of the code to be used	TURBO3D
Own code / 3rd party code?	Own code
Code publicly available?	Yes
Pure MPI or mixed OpenMP / MPI communication? Specific libraries	Pure MPI
On which machines is this code currently used for production runs, and how many cores are being employed?	JUROPA/HPC-FF ANIC5.ULB.AC.BE
Example for the strong scaling performance [fixed problem size] of the code	Linear scaling up to 64 nodes using an infiniband based cluster
Expected code scalability for the targeted problems in the present project	Max number of CPUs: 128

Review of previously studies that involved HPC...

Proposal for an IFERC-CSC Project

(for the **Project cycle 3** from 15th November 2013 to 14th November 2014)

- **Project Title** - ***Effects of Subgrid-scale TUrbulence on Particle Acceleration***
- **Project Acronym** - *ESTUPA*

Team: Bernard Knaepen *(ULB)*, Lapo Bettarini*(ULB)*, *M. Negrea (UCv)*, *I. Petrisor (UCv)*.

- **Types of Requirements**
- Computer resource requirements: Total amount of CPU hours: + 800 000

... The aim of our proposal is to study particle transport and acceleration in magnetic fields from highly accurate direct numerical simulations (DNS) of magneto-hydrodynamics (MHD) systems. The purpose is to relate the particle diffusion-coefficient properties to the characteristics of the electromagnetic fields and to study the influence of small-scale structures on particle transport and to mimic their role in more realistic closed models...

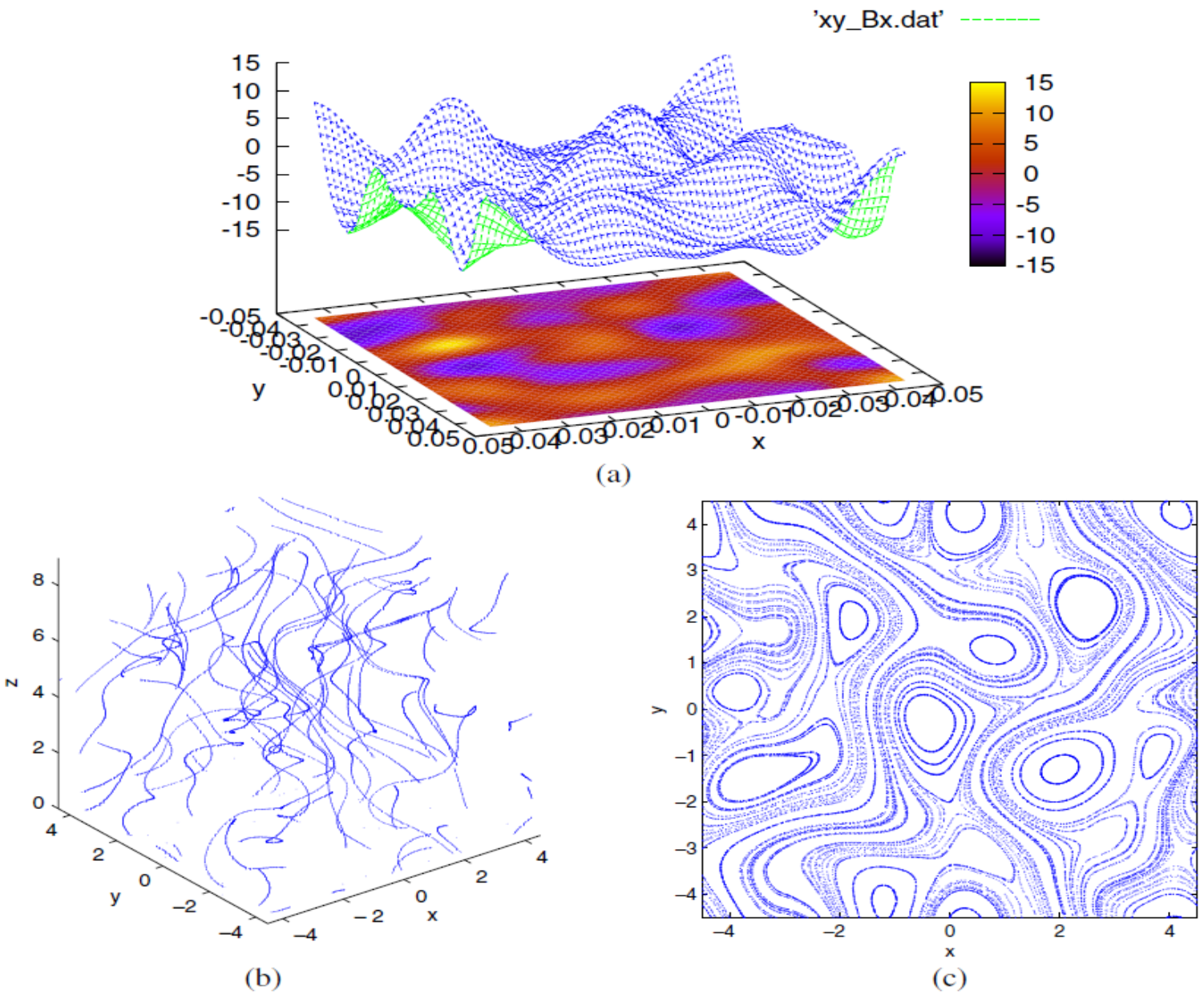

Figure 6. Shown are (*a*) the fluctuating magnetic field component b_x as a function of x and y for fixed z, (*b*) field lines in three-dimensional space and (*c*) field lines projected onto the x–y-plane for $z = \text{const}$.

Teams/peoples/needs

involved in large computations… under EURATOM/EUROFusion Program

- At least *5 teams* … theoretical physics groups…

Info..

In cadrul Integrated Tokamak Modelling Task Force (EFDA ITM-TF) – EURATOM Fuziune, la care participam de cativa ani (Colectivul "Modelarea matematica a plasmelor de fuziune" din INFLPR) la modelarea numerica a plasmelor tokamak descriptibile prin modele MHD (instabilitati de tip tearing, instabilitati rezistive de perete RWM, echilibru MHD in medii magnetice neliniare, etc.). Modelele de calcul sunt elaborate tot de noi in cadrul EFDA Topical Group MHD. Atat modelele cat si calculele noastre se refera la instalatii tokamak reale: ASDEX_Upgrade si JET. In ambele activitati, teoretice si de calcul, colaboram intens si de mult timp cu ***Institutul Max-Planck de Fizica Plasmei din Garching bei Munchen***, beneficiind de intreaga lor dotare de calcul performant. Aceasta este alcatuita din:

High Performance Computing:

- - IBM Blue Gene/P
- - IBM pSeries Power6 system (calcul paralel)

Capacity Computing: - Linux Compute Clusters (based on Intel Xeon and AMD Opteron processors for general purpose and dedicated computation)

- + facilitatile de calcul ale EURATOM Fuziune – **clusterul GATEWAY** din Italia.

Teams/peoples/needs

involved in large computations… under EURATOM/EUROFusion Program

- At least *5 teams* … theoretical physics groups…

Info..

- In cadrul Integrated Tokamak Modelling Task Force (ITM-TF), a fost dezvoltat un **portal de acces la resursele oferite de cluster-ul ITM Gateway**. In acest scop, au fost utilizate o serie de masini virtuale care asigura integrarea cu sistemul de autentificare si autorizare specific cluster-ului, precum si gazduirea si accesul la coduri de fuziune care au fost puse la dispozitia **task force-ului**. In plus, au fost dezvoltate o serie de aplicatii ale caror date sunt stocate intr-o baza de date de mari dimensiuni, gazduita in sistemul paralel de fisiere al cluster-ului. Printre acestea se numara "**ITM Catalog Querying Tool**", care realizeaza o interfata disponibila atat pentru utilizatori cat si pentru integrarea directa cu alte aplicatii.
- In cadrul proiectului **ITM AMNS** (Atomic, Molecular, Nuclear and Surface Data - **realizarea unei structuri de baze de date, cu un mecanism specific de acces**, care urmeaza sa fie utilizata in coduri masiv paralele ce urmeaza a fi rulate intr-o prima faza pe ITM Gateway si pe structuri tip GRID.

Resurse de calcul locale INFLPR: *Server dezvoltare si testare*: IBM BladeCenter S, 1xStorage Module, 1xblade HS22V (Code development for integrated modelling)

Resurse de calcul locale UCv: *Server testare*: Fujitsu Siemens

- **Resurse de calcul disponibile:** International Fusion Energy Research Centre (IFERC- CSC) (http://www.iferc.org/)

Teams/peoples/needs

involved in large computations… under EURATOM/EUROFusion Program

EURATOM Romania (2000 -2013) → **2014:** Consortiul **EUROFusion**

IFA structura reperezentativa in cadrul consortiului:

- **(INFLPR) Institutul National de Cercetare-Dezvoltare pentru Fizica Laserilor, Plasmei si Radiatiei**
- **Celelalte institute…**
- **Universitatile partenere…**

- Link util: **http://www.ifa-mg.ro/euratom/**

Teams/peoples/needs

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Intrebari:

- **Isi permite ROMANIA acces implicit si direct la resurse de calcul (pt cercetatori)?**
  In cat timp? Pt cat timp? Modalitati de eligibilitate?

- **Se obtine/acorda access la resurse de calcul <u>continuu</u>** pt cercetatorii din EURATOM/EUROFusion **(IP routabil, ssh, certificat digital + ssh dintr-un laptop mobil oriunde in lume?)**

- Cum se pot transfera 30 GB generate in simulari HPC de date daca este nevoie?
  (In cit timp, protocol SSH, etc…)