E-TASC / TSVV Task #13
Stellarator Turbulence Simulation
Kick off meeting

J. M. García Regaña

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 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Outline

I. Overview - Background and context of the TSVV Task 13

II. The TSVV#13 and the WPs W7X and AC.

III. The TSVV#13 and the ACHs

IV. The TSVV#13 work for 2021

V. Missions, communication and useful info.

VI. Summary

E-TASC within EUROfusion

- FP9 (*Horizon Europe*) has taken over Horizon 2020 as Multi-Annual Financial Framework (MFF) of the Comission for the period 2021-2027.
- EUROfusion Grant Agreement under FP9 (in preparation) has changes in the WP structure.
- New in EUROfusion ITER Physics Department: Theory and Advanced Simulation Coordination (**E-TASC**)

Theory & Advanced Simulation

The vision for the EUROfusion Theory and Advanced Simulation Coordination (E-TASC) is to integrate the world-class fusion science and engineering with emerging advanced computing capability. To this end,

1) JET
2) MST
3) Divertor Test Tokamaks
4) Plasma Facing Components
5) Stellararor Research
6) JT60-SA
7) Theory & Advanced Simulation

TSVVs within E-TASC

- A list of 14 **Theory Simulation Validation and Verification (TSVV) Tasks** addressing high-priority issues was ellaborated.
- Each linked to a *partner* WP.
- Call for participation (CfP) launched in May 2021.
- **0.5 ppy** minimum involvement.
- Participants: scientists + experts in computer science from Advanced Computing Hubs (ACHs).

Dep.	WP	#	Title
FSD	TE	1	Physics of the L-H Transition and Pedestals
FSD	TE	2	Physics Properties of Strongly Shaped Configurations
FSD	TE	3	Plasma Particle/Heat Exhaust: Fluid/Gyrofluid Edge Codes
FSD	TE	4	Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes
FSD	PWIE	5	Neutral Gas Dynamics in the Edge
FSD	PWIE	6	Impurity Sources, Transport, and Screening
FSD	PWIE	7	Plasma-Wall Interaction in DEMO
FSD	TE	8	Integrated Modelling of Transient MHD Events
FSD	TE	9	Dynamics of Runaway Electrons in Tokamak Disruptions
FSD	TE	10	Physics of Burning Plasmas
FSD	PrIO	11	Validated Frameworks for the Reliable Prediction of Plasma Performance and Operational Limits in Tokamaks
FSD	W7X	12	Stellarator Optimization
FSD	W7X	13	Stellarator Turbulence Simulation
FTD	DES	14	Multi-Fidelity Systems Code for DEMO

TSVV#13: Stellarator Turbulence Simulation
Resources: 7 ppy (70 % scientists, 30% ACHs)

TSVV#13 Stellarator Turbulence Simulation

What makes *Stellarator Turbulence Simulation* a high priority issue?

The understanding of turbulence in stellarators is limited in comparison to that in tokamaks.

- The **computational cost** of handling 3D geometries.
- The **limitations of the flux tube approach** for stellarators.
- **Electromagnetic turbulence** in stellarators is practically unexplored.
- The **interplay between neoclassical physics and gyrokinetic microturbulence**.

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TSVV Task 13: Stellarator Turbulence Simulation

Expected resources: Up to about 7 ppy per year (incl. about 30% for ACH personnel)

Background

Neoclassical processes have typically dominated radial energy transport in stellarators. However, as neoclassical transport is reduced in optimized stellarators, the turbulent component is expected to become essential to explain the total radial transport. This is confirmed by the results of the first experimental campaigns of Wendelstein 7-X, and it is true not only for the base plasma but also for impurity ions.

Gyrokinetics is the appropriate mathematical framework to describe turbulent transport in strongly magnetized plasmas. The field of gyrokinetic theory and simulations in stellarators is much less developed than in tokamaks. The flux-tube approach, valid for tokamaks, is questionable for stellarators because, due to the three-dimensional nature of the magnetic configuration, different magnetic field lines on a flux surface are not equivalent. Hence, codes that are qualitatively different from tokamak flux-tube codes must be built in order to correctly calculate stellarator turbulent transport. These codes must be stellarator-specific and formulated in a simulation domain that encompasses, at least, an entire flux surface. Only recently have supercomputers started to offer the computational power necessary to enable stellarator gyrokinetic simulations in full flux surface or fully global domains. In addition, there are also stellarator-specific neoclassical features that make things more complicated: the neoclassical distribution function, that can strongly depart from a Maxwellian, is a possible source of corrections to simpler gyrokinetic approaches.

Aims of the project

- Develop, verify, and validate a set of stellarator gyrokinetic codes going beyond the flux tube approach and self-consistently treating multiple particle species.
- Validate (and adapt, if needed) these codes for the calculation of turbulent fluxes in tokamaks with broken axisymmetry.
- Use these codes (and theory) to enhance the basic understanding of microinstabilities and turbulence in stellarators in different types of geometries and plasma conditions.

Key deliverables

1. Verified set of gyrokinetic stellarator codes that self-consistently treat multiple particle species (enabling, in particular, studies of turbulent impurity transport) and whose simulation domains cover an entire flux surface or a fully global domain. Assessment on the minimal simulation domain needed to correctly calculate turbulent fluxes and zonal flow dynamics in stellarators. Synergies with the tokamak community are to be sought.
2. Inclusion in (at least some of) these codes of the capability to use the neoclassical equilibrium as background distribution for turbulence calculations. Quantification of the modification of linear and nonlinear turbulence properties due to the neoclassical equilibrium.
3. Study of the relative weight of the neoclassical and turbulent branches of radial transport in multispecies stellarator plasmas, as a function of the species and the collisionality regime.
4. Validation of the codes for the calculation of turbulent fluxes in multispecies stellarator plasmas and in tokamaks with broken axisymmetry. In stellarators, explicit comparisons should be provided between the total transport experimentally measured and the sum of the simulated neoclassical and turbulent components.
5. Development of efficient reduced models (suitable for integration into stellarator optimization codes, see TSVV Task 12) capable of reliably predicting stellarator turbulent fluxes.

EUROfusion
Programme Management Unit
Boltzmannstr. 2
85748 Garching
Germany

EUROfusion
Programme Management Unit
Culham Science Centre
OX14 3DB Abingdon
United Kingdom

info@euro-fusion.org
www.euro-fusion.org

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TSVV#13 Stellarator Turbulence Simulation

Key deliverables by 2025

1. A set of **verified gyrokinetic stellarator codes**.
2. Capability of addressing the **interaction between neoclassical and gyrokinetic physics**.
3. Assessment of the **relative weight of neoclassical and turbulent transport**.
4. **Validation** of gyrokinetic codes for **stellarators** and **tokamaks with broken axisymmetry**.
5. Development of **reduced models**.

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TSVV Task 13: Stellarator Turbulence Simulation

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Proposal for TSVV#13

- **9 leading experts** in gyrokinetic theory and numerics. Developers and experienced users of the main European stellarator gyrokinetic codes + a neoclassical code.
- **Codes**: `stella`, `GENE`, `EUTERPE`, `GENE-3D`, `KNOSOS` (for NC input).

Member	Research Unit	Period	Commitment (ppy/year)
José M. García-Regaña (Task Leader)	CIEMAT	2021-2023	1.0
Edilberto Sánchez	CIEMAT	2021-2023	0.5
José Luis Velasco	CIEMAT	2021-2023	0.5
Michael Barnes	CCFE (Uni. Oxford)	2021-2023	0.5
Félix I. Parra	CCFE (Uni. Oxford)	2021-2023	0.5
Alejandro Bañón-Navarro	MPG (IPP-Garching)	2021-2023	0.5
Jorge Alcusón	MPG (IPP-Greifswald)	2021-2023	0.5
Jörg Riemann	MPG (IPP-Greifswald)	2021-2023	0.5
Josefine H. E. Proll	DIFFER (Uni. Eindhoven)	2021-2023	0.5
ACHs participants[1]	t.b.d.	2021-2023	2.0
Total resources			7.0

- **External experts**: R. Kleiber (IPP-Greifswald), M. J. Pueschel (Uni. Eindhoven), Denis St-Onge (U. Oxford)
- **Ph.D. students (funded through WPTRED)**: A. González-Jerez, H. Thienpondt and F. J. Escoto from Ciemat, A. von Boetticher (Uni. Oxford), F. Wilms (IPP-Garching), … (please, informe me if someone must be included)

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Table 1: Milestones of the TSVV Task in chronological order. The responsible person for each milestone is indicated with the symbol * after his or her initials. Milestones beyond 2024 are indicative, precise plans for 2024 and 2025 will be defined and expanded in the course of the Task. MY.X denotes the X-th milestone of the Y-th year of the project.

Miles-tone ID	Short name	Brief description	Participants	Due date
M1.1	M-STELLA-COLL	Implementation of the full linearized collision operator in `stella`.	**MB*, FP**	Jul. 21
M1.2	M-BENCHMARK-ES-GLOB	Benchmark between `GENE-3D` and `EUTERPE` for electrostatic turbulence with adiabatic electrons.	**ES*, ABN, JR, JGR**	Jul. 21
M1.3	M-STELLA-FFS	Development of a full-flux-surface (FFS) version of `stella`.	**MB*, FP**	Dec. 21
M1.4	M-GENE-3D-EM	Development of an electromagnetic version of `GENE-3D` and	**ABN***	Dec. 21

➔ Milestones as major pieces of verification and code development.

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D2.1 / D-TURB-BULKTRANSP	1, 4	Dec. 2022
Motivation: In many experimental W7-X situations, the temperature and density gradient support both ITG and TEM driven modes, making important to address the question about their interplay.		
SMART deliverable: *(S) Study the turbulent transport of the main ions and electrons, including the nonlinear interplay between ITG and TEM turbulence in W7-X. (M) This will allow to anticipate fundamental features of the turbulence in W7-X OP2 plasmas. (A) The work will be carried out by ABN* with GENE−3D, ES and JR on the EUTERPE side. Flux tube simulations with stella, by MB and JGR, or GENE, by JA and JR, are also foreseen. Neoclassical input of the radial electric field will be provided by JLV with the code KNOSOS. (R) Comparisons of nonlinear GENE-3D and EUTERPE cases with adiabatic electrons have been successfully conducted already, nonlinear simulations with kinetic electrons have begun with EUTERPE, and flux tube simulations are routinely performed with stella and GENE. (T) Due date: Dec. 2022.*		
D2.2 / D-NUM-DIAG	**1, 4**	**Dec. 2022**
Motivation: The lack of dedicated synthetic diagnostics that appropriately translate the numerical output to the exact experimentally diagnosed quantities, geometry, accessible range of measurement, etc. prevents from an accurate experimental interpretation		
SMART deliverable: *(S) Development of synthetic diagnostics that provide meaningful numerical input for the interpretation of OP2 turbulence data. To start, support to the Doppler Reflectometry (DR) systems and Phase Contrast Imaging (PCI) systems is foreseen. (M) This will improve qualitatively the interpretation W7-X turbulence experimental data. (A) The work will be carried out by ES* with EUTERPE, JA with GENE and JGR with stella. (R)*		

➔ Milestones as major pieces of verification and code development.

➔ SMART deliverables that contribute to a least one of the key deliverables of the CfP.

- **External experts**: R. Kleiber (IPP-Greifswald), M. J. Pueschel (Uni. Eindhoven), Denis St-Onge (U. Oxford)
- **Ph.D. students (funded through WPTRED)**: A. González-Jerez, H. Thienpondt and F. J. Escoto from Ciemat, A. von Boetticher (Uni. Oxford), F. Wilms (IPP-Garching), … (please, informe me if someone must be included)

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- **Codes**: `ste` ... input).

D2.1 / D-TURB-BULKTRA
Motivation: In many exp... support both ITG and TE... their interplay.
SMART deliverable: *(S) S... including the nonlinear i... allow to anticipate fundo... work will be carried out b... simulations with* `stell`... *Neoclassical input of the ... (R) Comparisons of nonli... been successfully conduc... begun with EUTERPE, a... GENE. (T) Due date: Dec.*
D2.2 / D-NUM-DIAG
Motivation: The lack of ... numerical output to the ... range of measurement, e...
SMART deliverable: *(S) D... numerical input for the i... Doppler Reflectometry (D... (M) This will improve qu... The work will be carried ...*

...nes as major ...of verification ...de development. ...deliverables ...ntribute to a ...e of the key ...ables of the CfP.

- **External expe**...), Denis St-Onge (U. Oxford)
- **Ph.D. student**... dt and F. J. Escoto from Ciemat, ... ease, informe me if someone m...

E-TASC SB evaluation: 4.77/5 (Category 1)

- Scientific Excellence: 4.69/5
- Quality of the implementation 4.77/5
- Project Team: 4.92/5.

No proposal of modification, with just the comment:

Regarding the validation of the codes for tokamaks, WPTE will reach out to the tema to identify suitable validation opportunities

GA endorsement on 3/3/2021. Indicative budget of 1.15 M€, approx.

TSVV#13 and the E-TASC SB and WPs

- Each **TSVV** will be **treated as a project** under the respective PI.
- **All TSVVs and ACHs** will be hosted under the WP Advanced Computation (**WPAC**).
- **The TSVV will report to the E-TASC SB yearly (report and presentation of results by the PI)**. PLs and TFLs are represented and have special roles
- **The partner WP** of the TSVV-13 is **WPW7X**
  PL: A. Dinklage; Deputy PLs: I. Calvo and J. A. Alonso.
- **Pinboard clearance** will include, besides the TSVV **PI**, at least one **WP Leader**.

Pinboard clearance

- All **publications** based on results produced **with support from EUROfusion** must be cleared by the TFL, PI or equivalent.

- The **clearance procedure** ⇒ uploading the document to the electronic pinboard at least **2 weeks** prior the deadline for **non-refereed** conference paper or abstract, **3 weeks for refereed** ones:

https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/index.jsp

- In case **W7-X results or input** (e.g. VMEC equilibria) is used, results must be **presented to the W7-X Team** (W7-X Physics Meetings, Wednesdays at 14:30 CET) **and/or Topical Group**: *Impurity Transport* or *Turbulence (*once every two weeks*)*

The TSVV#13 and the ACHs

- **30% of the manpower** of the TSVV will be allocated to the ACHs.

- Our requests in the proposal
  - **GENE-3D**: implementation of a massively parallel multigrid solver and optimized preconditioners.
  - **stella**: characterize the current scalability of the code and optimize it, in preparation of the FFS version.
  - **EUTERPE**: support for advanced visualization techniques of the numerical output and support for the usage of high compression formats for data transfer.

The TSVV#13 and the ACHs

- **30% of the manpower** of the TSVV will be allocated to the ACHs.

- The 5 selected ACHs:

Name	Category	RU	PI
ACH-1	HPC	MPG (IPP-Garching)	R. Hatzky
ACH-2	HPC	EPFL	P. Ricci
ACH-3	HPC	CIEMAT (BSC)	M. Mantsinen
ACH-4	IMC	IPPLM	M. Plociennik
ACH-5	DM	VTT	F. Granberg

HPC = High Performance Computing (scalable algorithms, code parallelization & performance optimization, code refactoring, GPU-enabling etc.)
IMC= Integrated Modeling and Control (code adaptation to IMAS, IMAS framework development, code integration etc.)
DM = Data Management (open access, data management, data analysis tools, aspects of AI and VVUQ, etc.)

The TSVV#13 and the ACHs

- **30% of the manpower** of the TSVV will be allocated to the ACHs.

- In preparation for the **TSVVs/ACHs Kick off meeting**, to be held on 23rd of April:

Action#1 on TSVV PIs: provide specific input about the tasks required to ACH

TSVV	Code name	Tasks required to ACH	ACH name

Please provide your input before April 15th.

HPC = High Performance Computing (scalable algorithms, code parallelization & performance optimization, code refactoring, GPU-enabling etc.)
IMC= Integrated Modeling and Control (code adaptation to IMAS, IMAS framework development, code integration etc.)
DM = Data Management (open access, data management, data analysis tools, aspects of AI and VVUQ, etc.)

HPC resources

- 40% of the CINECA/Marconi for EUROfusion reserved for the TSVVs ➔ Call for Participation (CfP)
- TSVV got all the CPU time requested of ~60 Mhrs above the limit established by the CfP for a single project.
- **Prioritize the usage of the TSVV/Marconi over other project you may be involved (6.6 % spent already).**
- **Action#2**: contact me if you are not yet included among the users of the project.

Work space	**/marconi_work/FUA35_STELTURB/**
Scratch space	**/marconi_scratch/userexternal/**

EUROfusion

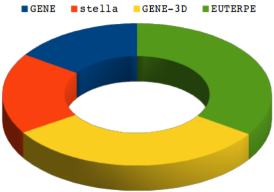
Proposal for the EUROfusion HPC 5th cycle / TSVV#13 Stellarator Turbulence Simulation

Proposal for a EUROfusion HPC Project

(for the **Project cycle 5** from 15th March 2021 to 28th February 2022)

Project Title	*Stellarator Turbulence Simulation*
Project Acronym (up to 8 characters)	*STELTURB*
Category [check the relevant research area(s)]	✓ Plasma turbulence and related transport processes Fast particle physics Linear, nonlinear and/or extended MHD Edge physics Heating and current drive Integrated modelling of fusion plasmas Reactor materials Reactor technology
Is this a continuation of a previous project?	No

Abstract



Milestones in 2021

Miles-tone ID	Short name	Brief description	Participants	Due date
M1.1	M-STELLA-COLL	Implementation of the full linearized collision operator in stella.	MB*, FP	Jul. 21
M1.2	M-BENCHMARK-ES-GLOB	Benchmark between GENE-3D and EUTERPE for electrostatic turbulence with adiabatic electrons.	ES*, ABN, JR, JGR	Jul. 21
M1.3	M-STELLA-FFS	Development of a full-flux-surface (FFS) version of stella.	MB*, FP	Dec. 21
M1.4	M-GENE-3D-EM	Development of an electromagnetic version of GENE-3D and implementation of methods that allow to use larger time steps in GENE-3D simulations.	ABN*	Dec. 21

*Each milestone/deliverable has a reponsible person for its coordination.

Deliverables in 2021

Deliverable ID / Short name	Key deliverable(s)	Due date
D1.1 / D-REF-CASES	1, 3, 4	March 2021
Motivation: The stellarator gyrokinetic community lacks **a reference case**, similar to the Cyclone Base Case (CBC) in tokamaks (…) Tokamak equilibria with broken axisymmetry will also be considered.		
SMART deliverable: (S) Agreed W7-X reference case and set of representative OP2 operation scenarios for comparisons, benchmark activities and OP2 predictive modelling tasks (…) JGR*(…) Due date: March 2021		
D1.2 / D-TURB-ZTRANSP	3, 4	Dec. 2021
Motivation: Due to the larger mass and charge of impurities (…) natural question about the effect of collisions on the turbulent transport of impurities.		
SMART deliverable: (S) Study of the effect of collisions on the background turbulence and impurity transport in multispecies electrostatic flux tube simulations (…) MB*, A. v. Boetticher (AvB, U. Oxford, PhD project), FP and JGR. (…) Due date: Dec. 2021.		

*Each milestone/deliverable has a reponsible person for its coordination.

Deliverables beyond 2021: W7-X campaings

- **Numerical support for W7-X turbulence related results** in next campaigns (starting by late 2022 or beginning of 2023) **will rest** in big extent in our TSVV.

D3.3 / D-SUPPORT-OP2.1	1, 2, 3, 4	Dec. 2023
Motivation: Once the first OP2 campaign has finalized (…) support of the experimental analyses and the interpretation (…).		
SMART deliverable: (S) Theoretical support and numerical simulations for W7-X OP2 (…) be partly accomplished by Dec. 2023, although it is likely that the analyses extent along 2024 too.		

D4.1 / D-SUPPORT-OP2.2	1, 2, 3, 4	Dec. 2024
Motivation: In a way similar to D-SUPPORT-OP2.1 (…) support of the experimental analyses and the interpretation (…)		
SMART deliverable: (S) Theoretical support and numerical simulations for W7-X OP2.2 discharges (…) partly accomplished by Dec. 2024.		

*Each milestone/deliverable has a reponsible person coordinating it.

Deviations and risk assessement

- If **deviations** from initial plan are expected, please, **inform the PI** so that:
  - a **correction measure** can be applied.
  - the PMU knows in advance and introduce, if possible, an **ammendment to the Task Agreements (TA)**.
  - The E-TASC SB is informed of that deviation in advance.

Table 3: Risk assessment table, considering the main risks for the development of the TSVV task identified at present and possible mitigation measures. Risk index color scale 1-9 (low), 10-15 (moderate), 16-25 (high).

Risk	Proba-bility (1-5)	Impact (1-5)	Risk index (1-25)	Mitigation	Risk index after mitigation
Milestone related to code development is delayed.	1	3	14	Regular reporting and review of progress on the different milestones in order to anticipate, if necessary, the realization of some deliverable, or parts of it, with other codes within the TSVV.	9
Insufficient assigned CPU hours in Marconi	3	4	16	Application for computing time to instances other that EUROfusion, e.g. the Spanish HPC Network (RES, Spain) and other national agencies, PRACE, etc.	9
Team member leaves the TSVV.	1	5	20	Recruitment of a substitute with similar competencies and expertise. Communication to the PMU for modification of the TAs, if necessary.	12
OP2 campaigns suffer delays	2	3	22	Mitigation measures are out of the domain of the Task. Other activities could be strengthened in order to back up the validation and campaign support activities: participation in LHD through international collaborations, MST or TJ-II.	15
COVID-19 crisis worsens, restricting travels, increasing childcare load, postponing conferences, etc.	3	4	22	Mitigation measures are out of the domain of the Task. The status of the different milestones and deliverables should be precisely tracked in order to give feedback to EUROfusion to postpone missions or usage of manpower resources according to the estimated delays.	16

TSVV-13 Missions

- The plan for **missions** is **not yet confirmed** by the PMU.
- **Missions to W7-X** site are expected to be funded through the **WPW7X budget** for campaign visits.
- **Travels** within Europe for **meetings among the team members** will be funded through a dedicated **mission budget** within **WPAC** and approved by the Scientific Secretary of WPAC.
- **About international missions** or **collaborations no information has been provided, PIs** have been asked **to provide input.**

⇒ **Experimental validation → non-EU devices:** LHD (NIFS, Japan), HSX (Uni. Wisconsin, USA), CFQS (Southwest Jiaotong University, China)

⇒ **Code verification → non-EU codes:** GKV (NIFS, Japan), XGC (PPPL, USA), etc.

TSVV-13 logistics and useful info

- A wiki, whose mantainance and update is responsability of the PI, has been set up:

  https://wiki.euro-fusion.org/wiki/TSVV-13

- Indico repository for presentations:

  https://indico.euro-fusion.org/category/286/

- To login the two sites, the credentials are those of your EUROfusion IMS account, which is also used for mission application

  https://ims.euro-fusion.org/

⇒ **Action#3**: apply for an IMS account if you do not have one.

TSVV-13 logistics and useful info

- **Zoom** will be the VC tool used for remote meetings of the team and external experts.
- **Remote meetings** on a **monthly** basis (is it OK this slot, Monday, 15:00-16:00 CET?)

  Purpose: share the results obtained along the deliverables and milestones of the project, get feedback from external participants, **everyone knows what the others are doing**, etc.

- **Meetings at the level of working groups** involved in specific work pieces can be held **on demand** of the interested team members.

- For **rapid** information flow and **communication**: email, phone, Telegram. Contact details of all the team will be available on the wiki, **is that OK?**

Summary

- **TSVV** begins on **first or April** and will extend over a 5 year period with a total funding of 1.15 M€ approximately.
- Task Agreements with final budget figures are under preparation.
- Detailed mission management, monitoring and communication with partner WPW7X, ACHs, etc. to be provided to TSVV PIs on 23rd of April at kick off meeting.
- **Actions**

#	Action	Responsible	Due date
1	Provide specific input about the tasks required to ACHs	JGR	15th of April
2	Resquest to join the TSVV/Marconi Project STELTURB by sending me an email if not included yet.	All Team members	ASAP
3	Apply for an IMS account if you do not have one, necessary to access the project WIKI, application of missions, etc.	All Team members	ASAP

Questions?