EUROfusion

FZJ focuses and plans

FP-9: TSVV Task 5 *"Neutral Gas Dynamics in the Edge"*

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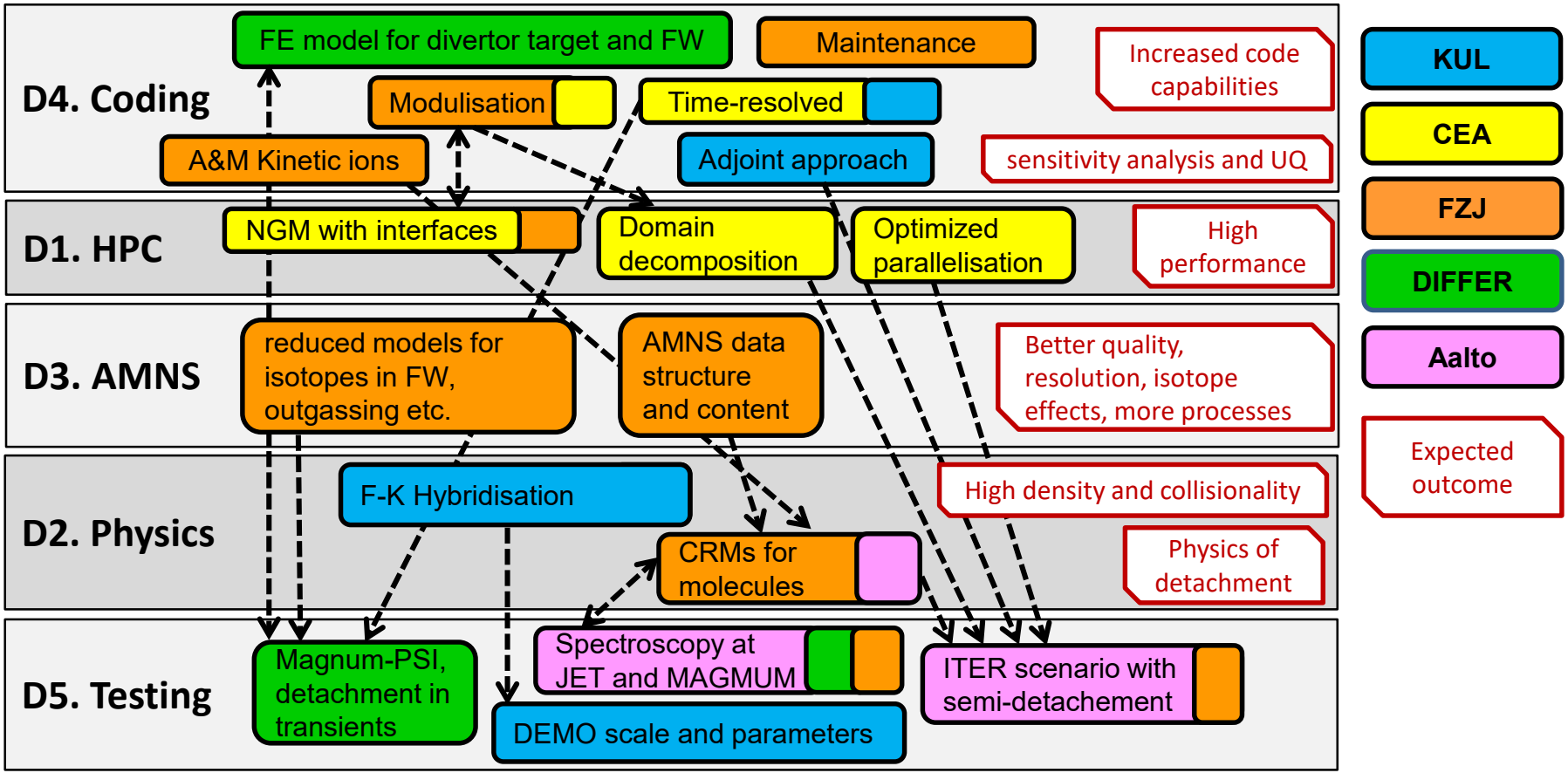
Crude scheme for the TSVV-5 workflow



Crude scheme for the TSVV-5 workflow

D4. Coding

A&M Kinetic ions

Collisional-radiative models **(CRMs)** including for molecules and **detachment,** also including photon tracing (**opacity**) are the central activity as well as **AMNS** data

D1. HPC

D3. AMNS

reduced models for isotopes in FW, outgassing etc.

AMNS data structure and content

D2. Physics

CRMs for molecules

D5. Testing

Spectroscopy at JET and MAGMUM

ITER scenario with semi-detachement

KUL

CEA

FZJ

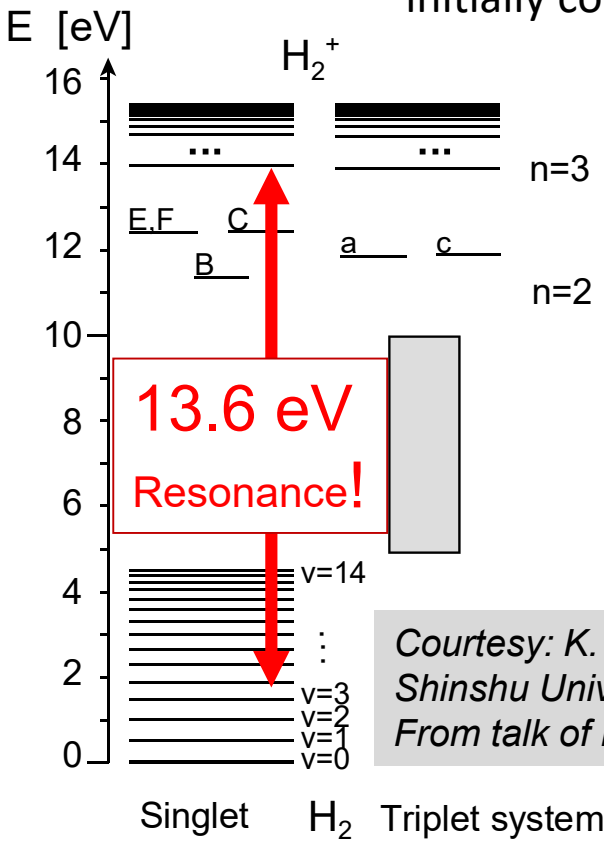
DIFFER

Aalto

H_2, present status in EIRENE:

➔ *D_2 (T_2, DT?..) needed!*
➔ *Resolution by T_{rot}, T_{vib} needed!*

initially compiled **1997**

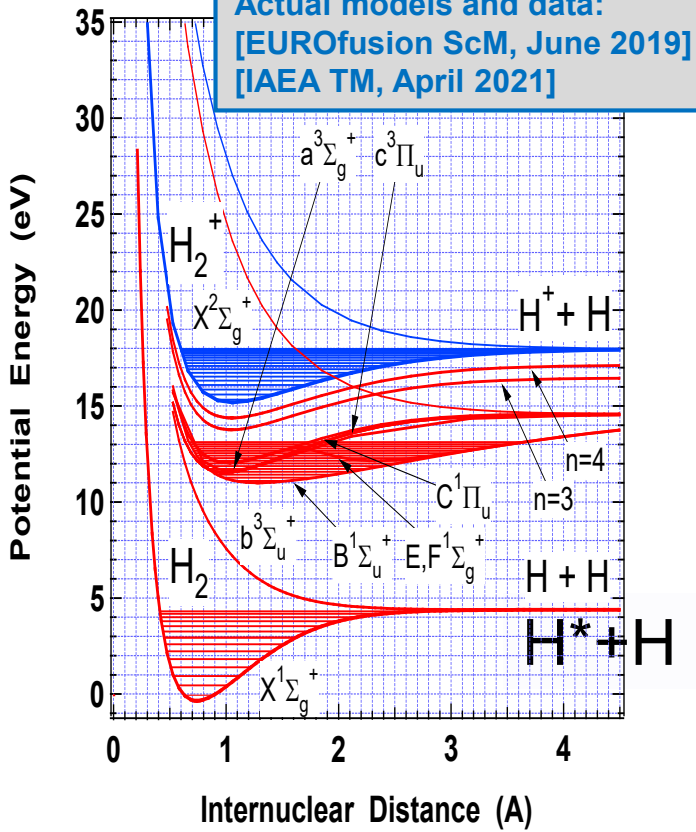


New models available recently!

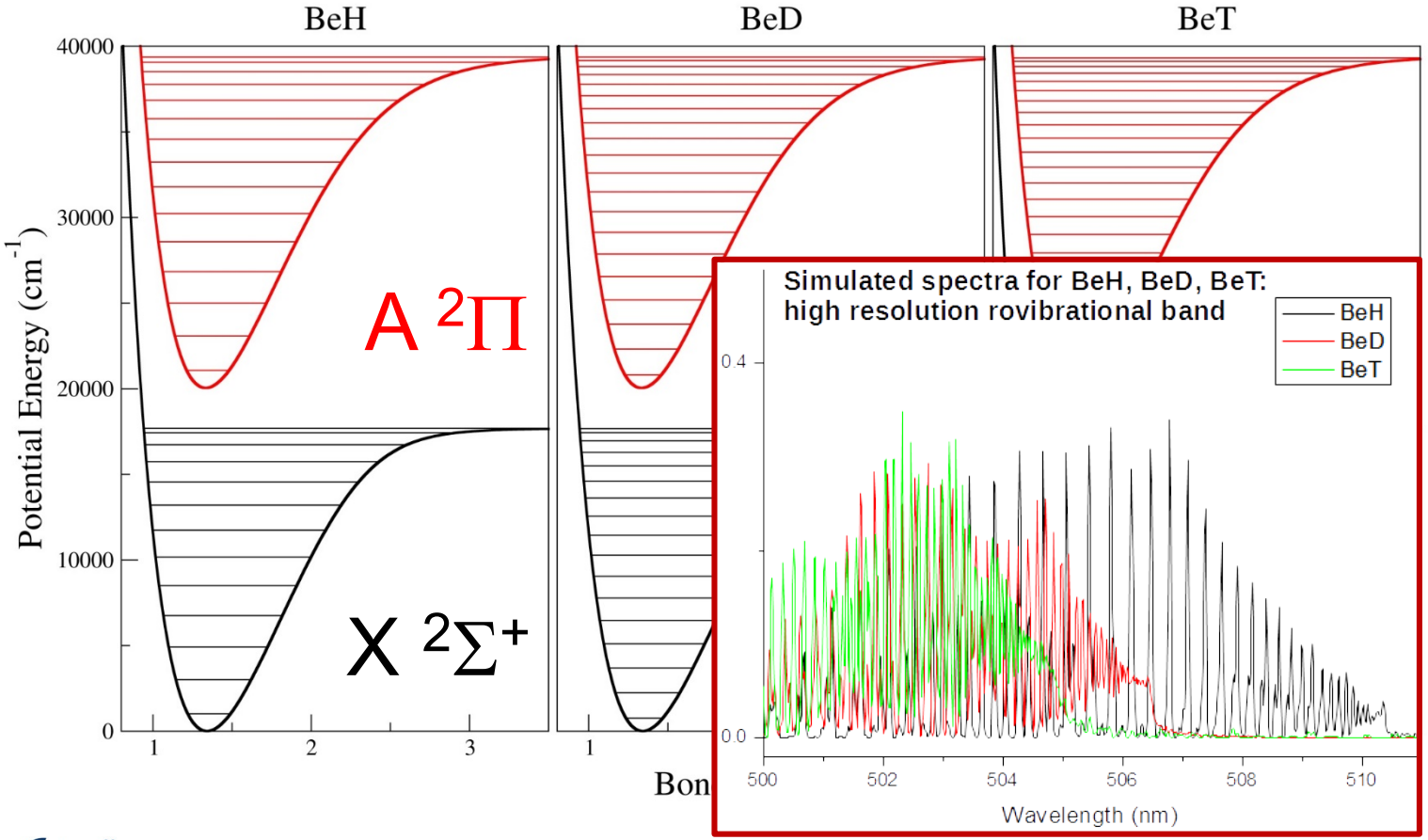
- → **ADAS "mdf" formats …**
- → **R-matrix and CCC data for molecules**
- → **Sawada for D_2**

Courtesy: K. Sawada, Shinshu Univ. Jp. From talk of D.Reiter

Actual models and data:
[EUROfusion ScM, June 2019]
[IAEA TM, April 2021]



Spectroscopic model for BeH/BeD/BeT



Strong isotopic effect!

J.Tennyson SCM talk

D. Darby-Lewis, et al.,, Synthetic spectra of BeH, BeD and BeT for emission modelling in JET plasmas, *J. Phys. B: At. Mol. Opt. Phys.*, **51**, 185701 (2018)

Crude scheme for the TSVV-5 workflow

D4. Coding

Modulisation

Maintenance

D1. HPC

NGM with interfaces

D3. AMNS

EIRENE-NGM restructuring and maintenance should remain a significant effort for the FZJ team!..

D2. Physics

D5. Testing

KUL

CEA

FZJ

DIFFER

Aalto

FZJ contributions (central to the TSVV-5!)

	ID	RU	
D1. Code performance, refactoring parallelization, HPC, …	D1.a	CEA/FZJ	Code development (interfaces, refactoring, HPC), main effort on CEA
	D1.b	CEA	
	D1.c	CEA	Domain decomposition and **parallelization**
	D1.d	KUL	adjoint approach
D2. Improved physics and features incl. FKH and CRM	D2.a	KUL+CEA	
	D2.b	KUL	F-K hybridisation
	D2.c	FZJ/Aalto	**Improved CRMs** (ro-vibrational temperature, isotopes, photon tracing)
D3. Improved AMNS data, both in structure/physics and content	D3.a	FZJ/ACH IM	
	D3.b	FZJ/ACH D	**AMNS data** structure and content. New, after 2024: reduced models for PSI (outgassing, CAPS, isotopes in FW, . . .)
D4. EIRENE as NGM – restructuring, interfaces to other codes, time-dependent runs	D4.a	CEA/KUL	
	D4.b	DIFFER	
	D4.c	FZJ/CEA	Code **restructuration**, additional specific modules
	D4.d	FZJ-leading +All	Versioning, portfolio of simulation cases, etc . . .
D5. Validation with experiments and test of predictive capabilities	D5.a	Aalto/ DIFFER/FZJ	CRM, AMNS validation at JET and DIFFER
	D5.b	DIFFER	Validation at MAGNUM of FE model and data for PSI
		KUL	Demonstration of FKH advantages for DEMO
	D5.c	Aalto/FZJ	ITER-relevant physics for **detachment** extrapolation from JET to ITER

In red: good research focus for D.Borodin + PhD-student/postdoc

Area of FZJ expertise, highlight for decades. May look routine, but lots of valuable physics inside!..

DB view: yes, community service, however FZJ team is willing to keep the lead in this!..

ACH D support is expected

FZJ contribution: suggested commitments

ID	RU
D1.a	CEA/FZJ
D1.b	CEA
D1.c	CEA
D1.d	KUL
D2.a	KUL+CEA
D2.b	KUL
D2.c	FZJ/Aalto
D3.a	FZJ/ACH Hub
D3.b	FZJ/ACH D
D4.a	CEA/KUL
D4.b	DIFFER
D4.c	FZJ/CEA
D4.d	FZJ-leading +All
D5.a	Aalto/ DIFFER/FZJ
D5.b	DIFFER
	KUL
D5.c	Aalto/FZJ

Topic / Commitment	DB	PhD/postdoc	Comp. scientist or MaTSE
Code development for HPC: NGM interfaces to other TSVV codes, road to efficient parallelization, etc.	5%		5%
CRMs for molecules (Resolution by ro-vibrational states, isotopes, photon tracing)	25%	50%	?..
AMNS structure, content, link to advanced PSI through reduced models (>2024…)	20%	35%	30%
Central code development (general restructuring similar to ERO2.0: compact numeric core and "starter")	10%		30%
Basic code maintenance (versioning, simulation cases, etc.)	10%		35%
Code validation and predictions for **ITER**, physics of **detachment**	15%	15%	-
Leading TSVV-5, responsibility for EIRENE (NGM in future)	15%		
PPY in TSVV-5:	0.75	0.75	0.5

This plan provides reasonable human resources for EIRENE development!

WP DC + TSVV-5 postdoc position

"Improvement of A&M CRMs in the EIRENE-NGM for spectroscopy-based detachment control"

EUROfusion	Key research and EIRENE development items	PPY support
TSVV-5 (WP PWIE)	• Interface to **molecular CRMs in ADAS** including **refined models for D2/H2;** incorporating **new ADAS "mdf" formats.** • Providing **rovibrational temperature** as a parameter and **isotope effect**; incorporation and validation of the related data. • **Optimization of the CRM for speed** based on providing flexible approach for selection of appropriate states to be tracked. • Investigation of key **molecular processes in detached plasma;** analysis of preferable reaction chains using **classical eigenvector** approach as well as modern **nonlinear dynamics math approaches** • Validation at with **JET** and **MAGNUM-PSI**, extrapolation for **ITER/DEMO** (TSVV "portfolio" cases).	**0.75** for postdoc (or PhD-student) position **0.75** for PI including own scientific contribution
WP DC	• DEMO: predicting **spectroscopic emission characteristic for detachment** including from molecular species. • relating the light emission to degree of detachment; **detachment control**.	**0.3** for postdoc **0.2** for supervisor

FZJ part of the TSVV-5 team

Participant			Commitments, person per month (ppm)						
Name	RU	Role in TSVV-5	2021	2022	2023	2024	2025	2026	2027
Dmitriy Borodin	FZJ	Task Leader, Contact person FZJ, **senior scientist**, CRMs for molecules, AMNS, detachment, EIRENE as NGM: code development, validation and maintenance	9	9	9	9	9	9	9
Vacancy	FZJ	**Computer and IT engineer**, EIRENE as NGM: code development, validation and maintenance, support of AMNS database and web-services	6	6	6	6	6	6	6
Vacancy	FZJ	**PhD-student or postdoc**, CRMs for molecules, AMNS database structure and content, detachment	9	9	9	9	9	9	9

Considerable alternative: postdoc (with WP CD, detachment in DEMO) + PhD student (CRMs, surface data, application to JET and other experiments)

➔ *Hiring to fill the vacancies is urgent and priority task . . . It causes not just a lack of manpower, but also additional uncertainty.*

Thanks for the attention!

Expected participants and RU commitments

Particular names may change with time, but workload distribution between RUs is expected to keep mostly . . .

We need to fill the vacancies in time

→ *FZJ: PhD-student(s)+postdoc (7 years in total), focus on molecules in plasma*

→ *FZJ: EIRENE + infrastructure maintance: computer scientist*

Name	RU	Selary level	2021-2023	after 2023
Wouter Dekeyser	KUL	4	0,5	0,5
Bert Mortier	KUL	3	0,75	0,75
Dmitriy Borodin	FZJ	5	0,75	0,75
Computer scientist VAC	FZJ	2	0,5	0,5
New PhD-Student, Molecules	FZJ	3	0,75	0,75
Jorge Gonzalez Munoz	DIFFER	4	0,5	0,5
Yannick Marandet	AMU/CEA	5	0,5	0,5
Paul Genesio	AMU/CEA	5	0,5	0,5
Andreas Holm	Aalto	3	0,8	0,8
Mathias Groth	Aalto	6	0	0,2
Giovanni Samaey	KUL	6	0,2	0
Algorithmic improvement	IM Hub		0,25	0,25
NGM Parallelisation	HPC Hub		0,75	0,75
HUB support (general incl IMAS)	_Hub		0,25	0,25
		Total:	7	7
		Hub support:	1,25	1,25
		Hub support[%]:	17,85714286	17,85714286

RU - PPY	AMU/CEA	FZJ	KUL	DIFFER	Aalto
2019/20	1,6	1,4	1	0	0
FP-9 (2021+)	1	2	1,45	0,5	0,8
FP-9 changes after 2023			-0,2 (G.Samaey)		+0,2 (M.Groth)

2nd TSVV-5 computer scientist or PhD-student vacancy

EUROfusion	Key research and EIRENE development items	PPY support
TSVV-5 (WP PWIE)	• **Unification of the A&M data with other codes** e.g. with **CFDs, ERO**. • Refinement, validation and **extension of the break-up data for molecules** including identification of the related data sources • Incorporation of **automatic A&M database tests** for consistency, unphysical behavior etc. • **Reduced models for the PSI data** (CAPS, outgassing, etc.) • General improvement of EIRENE (as NGM), e.g. **numeric core segregation**, optimisation for HPC, **interfaces to CFD**, refactoring, … • General improvement and extension for the databases. • Verification on **CI cases**, **validation with experiments.** • **Maintenance and documentation** of EIRENE and its databases	**0.5** for computer scientist (or PhD-student?..) position **0.75** for PI including own scientific contribution
?..	**Other code maintenance** work?.. (EMC3?.. ERO2?..) **CFD-EIRENE Applications to JET, PSI-2/JULE-PSI or W7-X**? ITER?	**0.5** or some other funding needed…

Suitable only for a PhD-student ← → ***rather for a computer scientist***

PhD-student/Postdoc position proposal

“Extension and Refinement of the EIRENE Atomic and Molecular Database”

- *Funding scheme will determine a lot (one of the options: TSVV-5)*
- *EIRENE (and infrastructure) demands significant “work-in” time (>6 months)*
- *Flexible: one can select various combinations of bullets below (any 2-3 will make-up good PhD-work)*

1. **Interface to molecular CRMs in ADAS including refined models for D2/H2 – newly developed (not yet officially released) “mdf..” data formats similar to the well-established “adf..” ADAS datasets are to be read and used in EIRENE simulations. This means also respective changes in the code (e.g. providing more detailed structure of the species/states available for tracking in a particular EIRENE run).**
2. **Providing rovibrational temperature as a parameter and isotope effect in atomic and molecular simulations combining an option to use additional data sets where available together with a set of approximated corrections for the rest of the data.**
3. **Refinement, validation and extension of the break-up data for molecules including identification of the related data sources.**
4. **Unification of the A&M data with other codes e.g. ERO. The later already uses automated export for HydKin data. However, this positive experience has large room for extension and also should become bi-directional.**
5. **Optimization of the CRM for speed based on providing flexible approach for selection of appropriate states to be tracked (seamless from bundling of ionization states down to tracking the internal excited states (e.g. metastables). In general, this is an eigenvalue problem.**
6. **Incorporation of automatic A&M database tests for consistency, unphysical behavior etc. Providing of automatic test for the database in the frame of the code versioning (e.g. based on GitLab or JuBE – Juelich benchmarking environment provided by JSC).**
7. **Investigation of key molecular processes in detached plasma based on deep mathematical analysis of preferable reaction chains using classical eigenvector approach as well as modern nonlinear dynamics math approaches.**
8. **Reduced models for the surface data (CAPS, outgassing, etc.)**