SOLPS and PMI modeling

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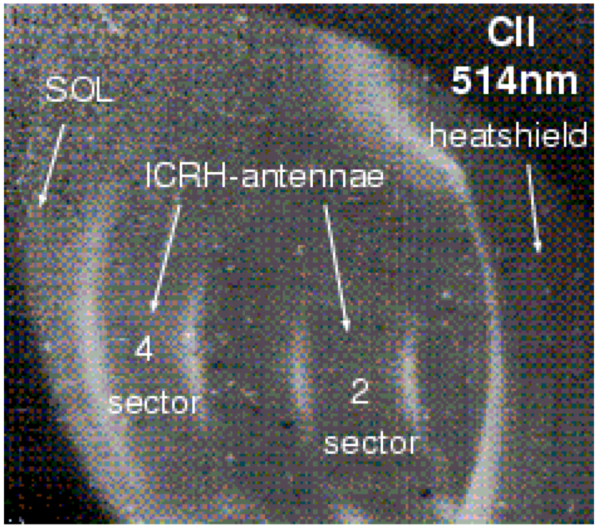
Contributors to the EFDA TF ITM

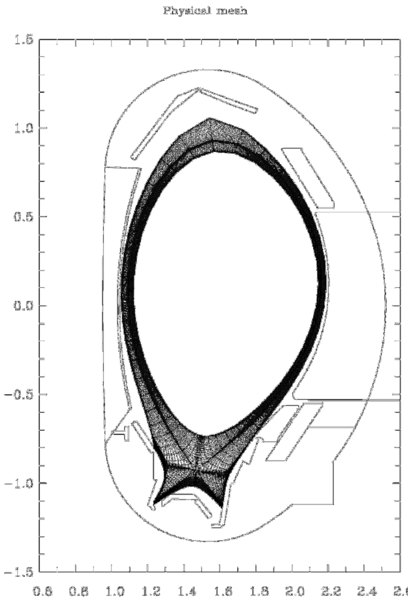
Introduction

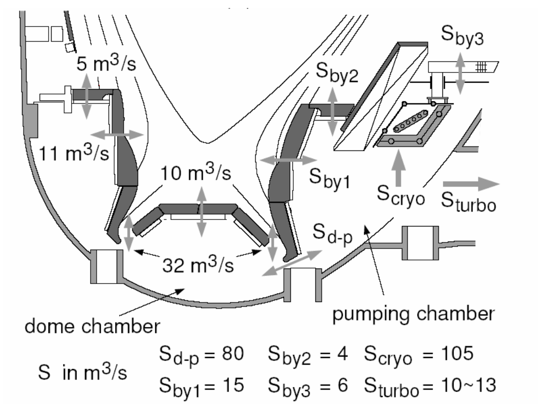
- what are the assumptions in the code (2d, fluid plasma, ...)
- what are the current developments (mixed materials, grid adaptation, better treatment of the drifts)
- what can be done to extend the calculation to the real wall (still assuming 2d)
- what are the developments in the EU with respect to code-code communication and AMNS data
- touch on missing physics and V&V

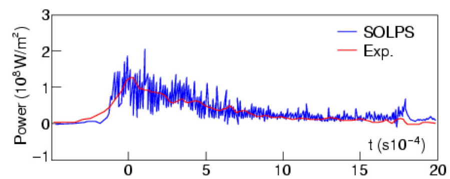
Assumptions/Limitations – Fluid, transport, 2d, domain, impurities, drifts, time-dependence

- Fluid treatment of the plasma
  - kinetic plasma effects not properly treated
    - Flux limiters
    - Should we investigate fluid/kinetic hybrids?
- Transport codes
  - No 1st principles treatment of radial transport
    - Radial and poloidal dependence of transport coefficients
    - Non-diffusive nature (+ pinches)
  - Parallel transport on a better footing (except for kinetic effects)
- 2D
- Solution domain somewhat limited
- Neutral treatment
  - Kinetic: coupling to a Monte-Carlo code
  - Fluid: usually not full Navier-Stokes
  - Often details of bypasses, wall out-gassing neglected
  - Neutral-neutral collisions and optically thick regions
- Impurities
  - Intrinsically produced
    - Somewhat simplified erosion/deposition models
  - Plasma solution domain usually doesn't extend to vacuum vessel
    - Problem with main chamber sources
  - PSI models usually too simple
    - Usually not affected by the plasma in the simulations
- Drifts
  - Still not complete agreement on the equations to be implemented
  - Not nearly as robust as the non-drift versions
- Time-dependent calculations
  - Still not that routine
  - Especially for detailed match to experiment



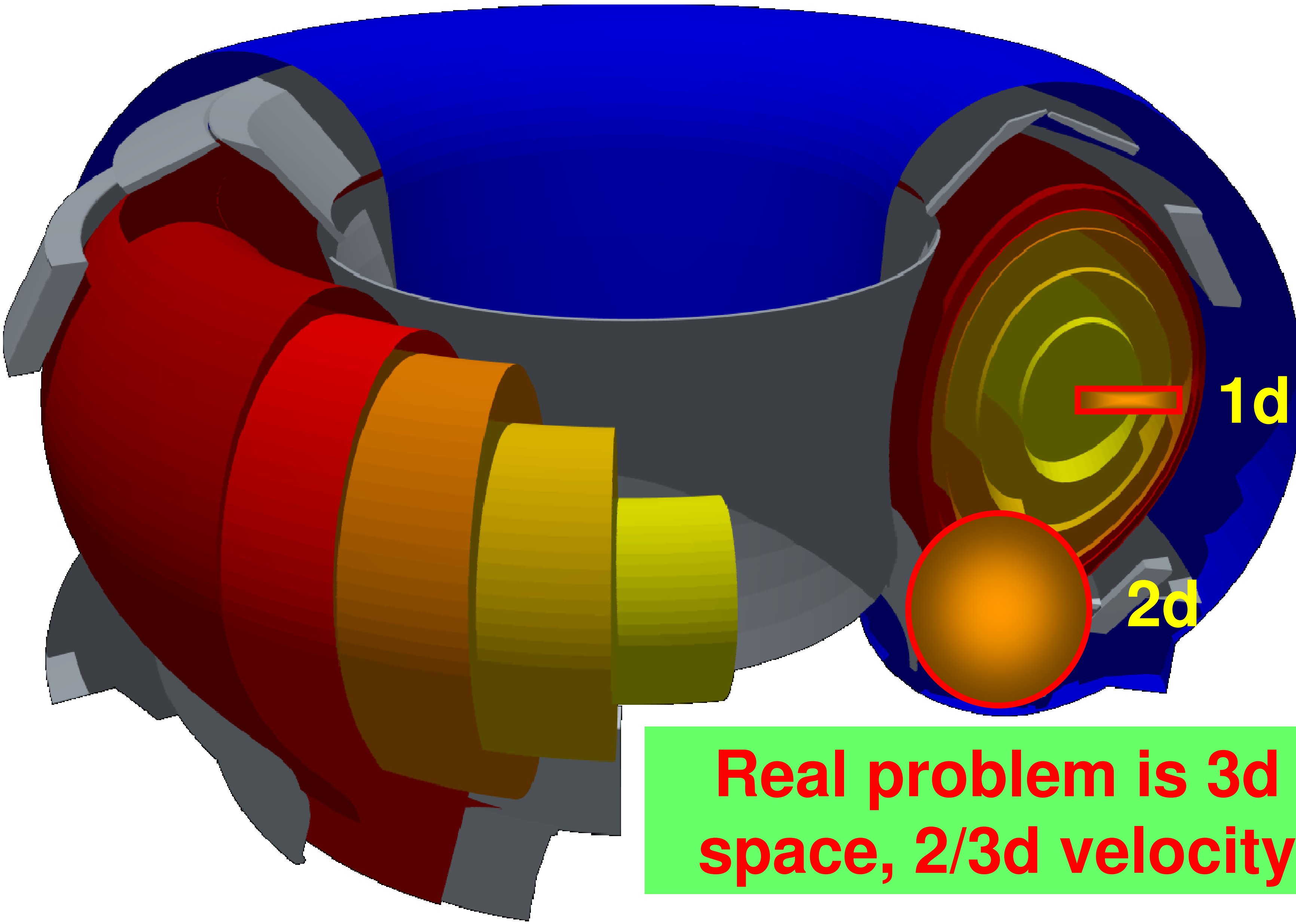






[Subba, EPS-2003]

Simulations

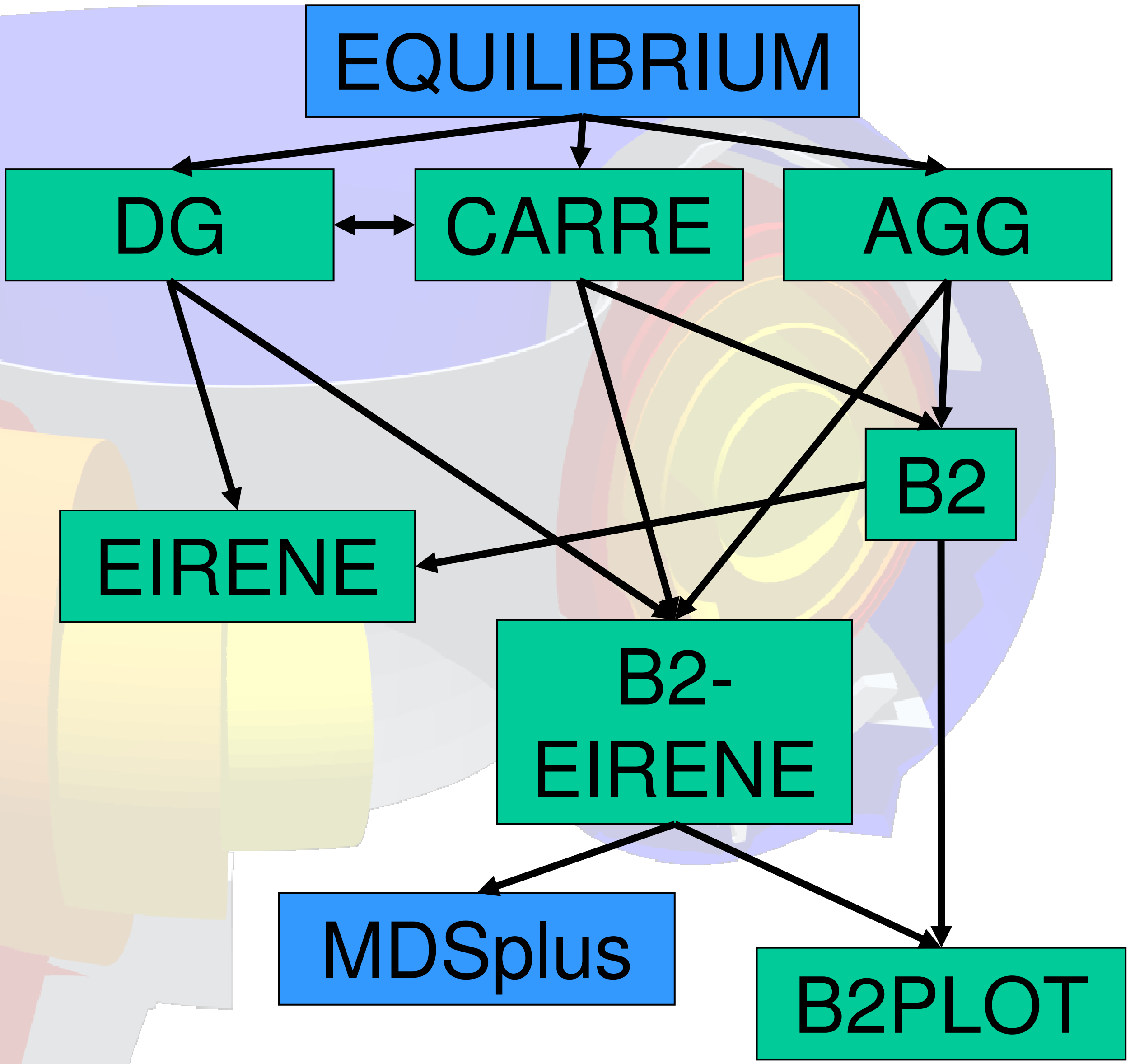


Real problem is 3d space, 2/3d velocity

What is SOLPS?

Suite of codes

- Grid preparation
  - CARRE
  - DG
  - AGG
  - (TRIANG)
- Plasma
  - B2, B2.5
- Neutrals
  - EIRENE
- Coupled
  - B2-EIRENE
- Visualization
  - B2PLOT

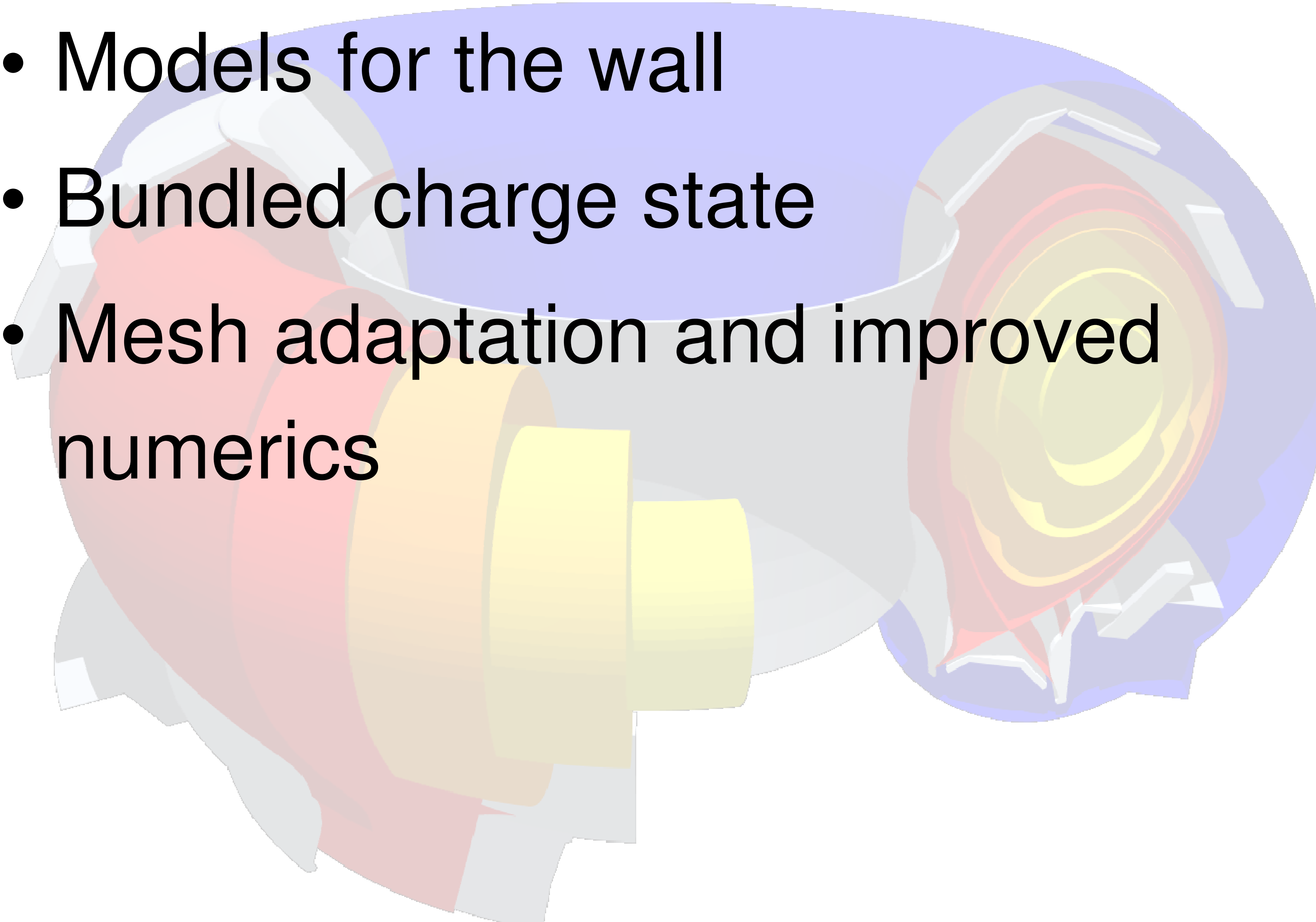


2d Edge Simulations

- Plasma
  - Fluid description
    - Density of ion charge states
    - Parallel momentum of ion charge states
    - Electron and ion temperatures
    - Potential

- Neutrals
  - Either
    - Fluid (2d)
    - **Kinetic** (3d mapped to 2d)
  - Include
    - Recycling
    - Volume Recombination
    - Sputtering
    - Gas puff and pump
  - With
    - Atomic physics
    - Molecular kinetics
    - Non-linear effects
      - Neutral-neutral collisions
      - Photon transport

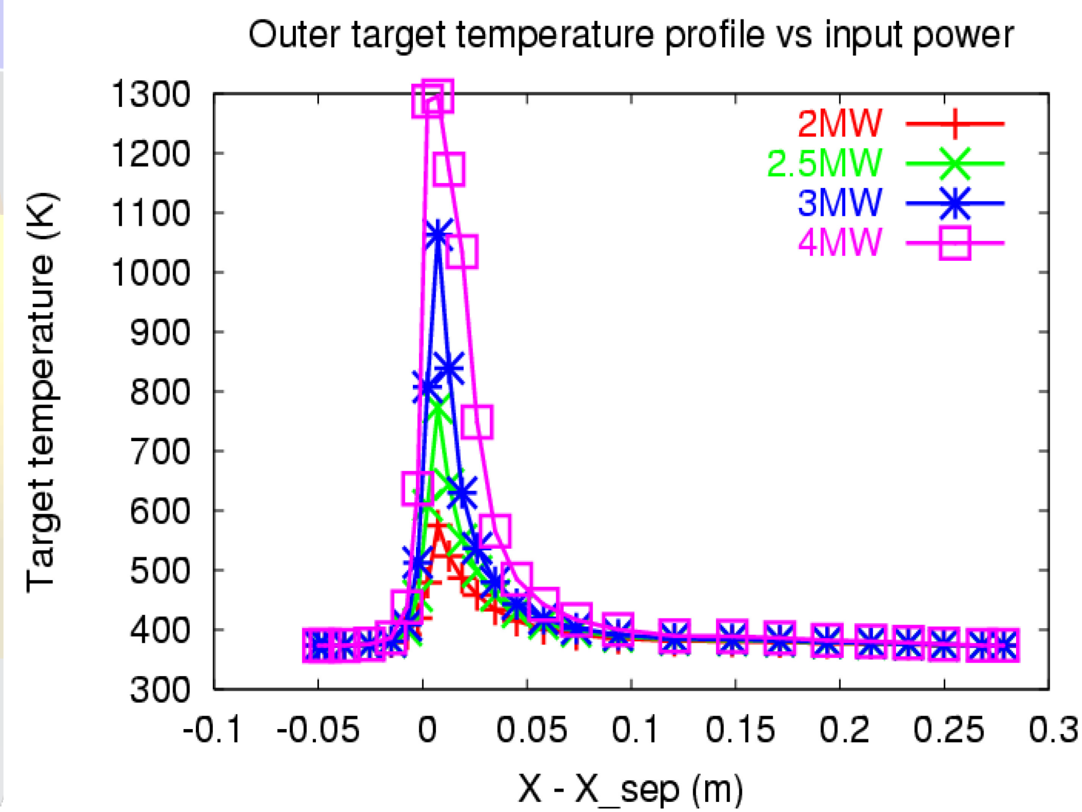
Current developments



- Models for the wall
- Bundled charge state
- Mesh adaptation and improved numerics

New developments

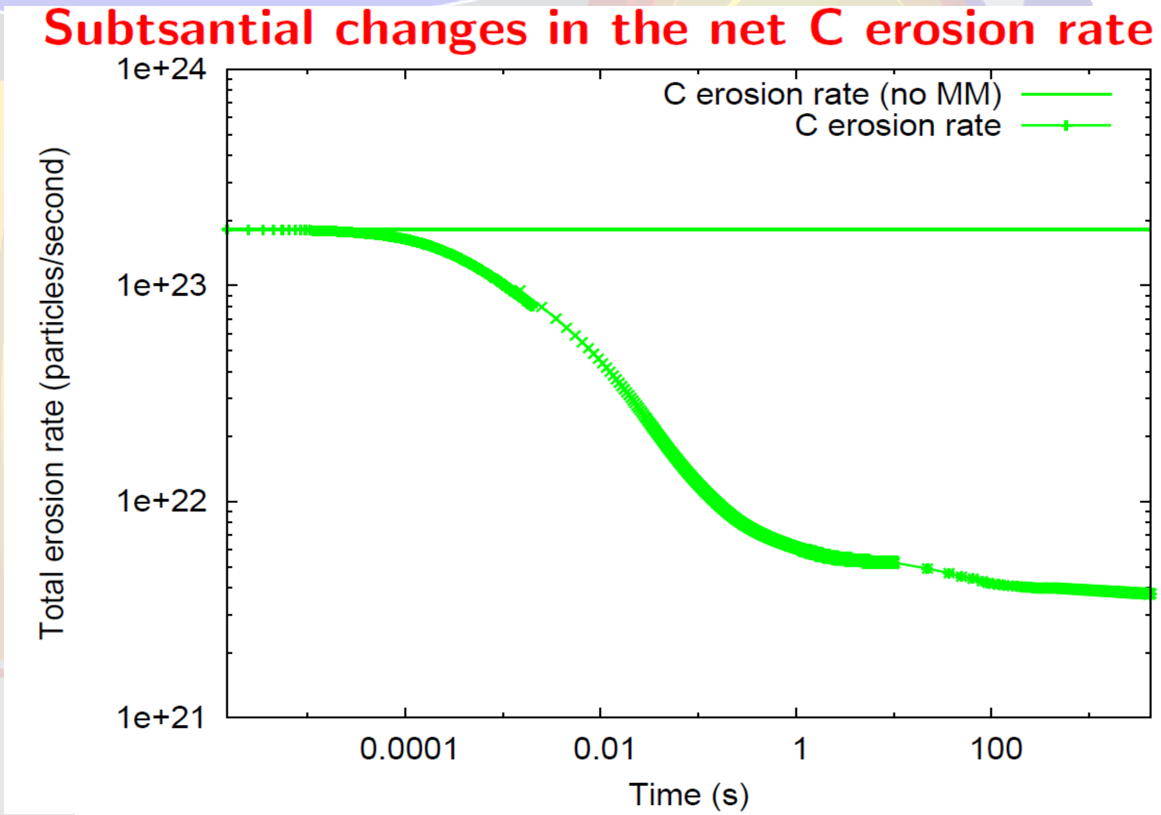
- Working towards more integrated models
  - Integrating plasma and plate
    - SOLPS5-B2
      - Fluid neutrals
      - Latest Roth chemical sputtering formula ==>
    - Working towards modelling mixed materials
  - Also integrating core and edge



New developments

- Current status:
  - Standardizing interfaces between various modules
    - Plasma
    - Neutrals
    - Wall
    - Main plasma
  - Will implement in CPOs (see later)

SOLPS5-B2 simulation of C erosion for an ITER simulation with C targets and Be walls



Exploration of W-bundling effects

Bonnin

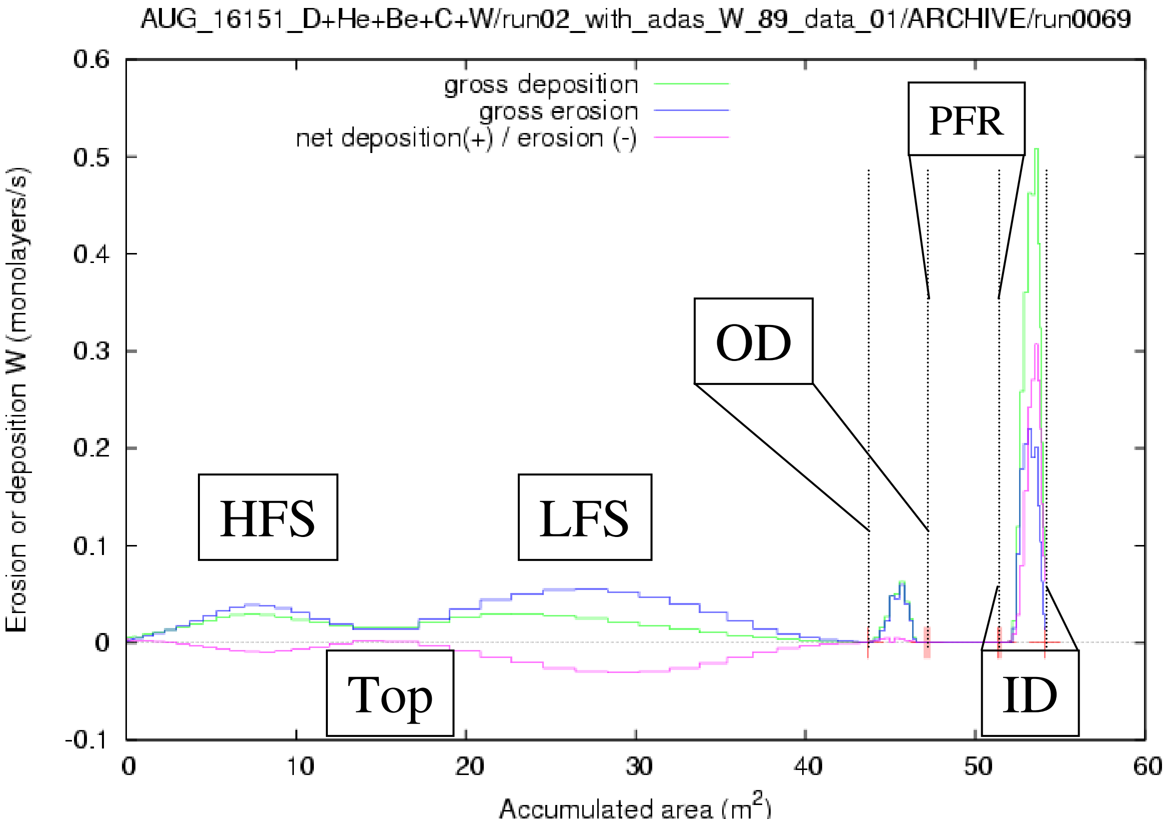
Name	Run #	ns
All	2	75
np	8	36
j2	6	27
t1	14	11
u1	17	11
v1	20	11
q	10	10
r	11	10
s	12	10
xb	22	23
xb_03	23	9
npj	9	27
j	5	27
itert	4	15
jett	7	24
tt	15	10
uu	18	10
vv	21	10
edg	3	10

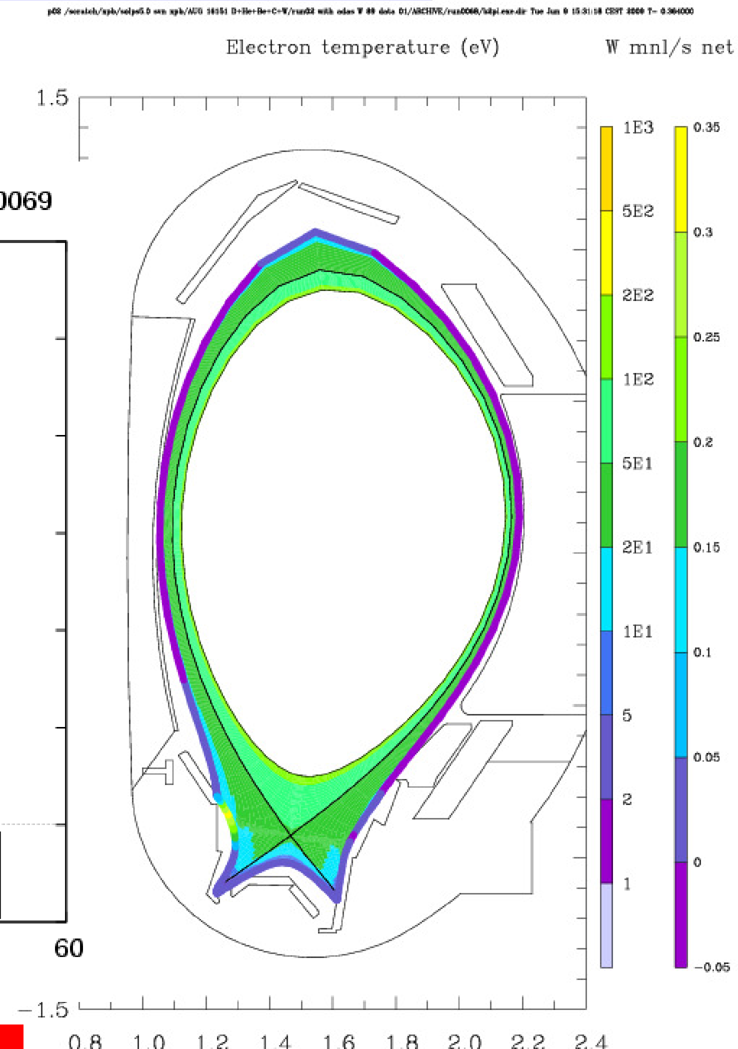
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
Configuration	W	Ta	Hf	Lu	Y	Tm	Er	Ho	Dy	Tb	Gd	Eu	Sm	Pm	Nd	Pr	Ce	La	Ba	Cs	Xe	I
	6s		5d				4f	5p						4f			5s					

- 17 different bundlings (only relevant low-level ionization stages shown, no significant densities above W^{+20} [Xe-like] in the plasma edge)
- From including all species to only 9 bundles (factor 4 total speed-up)
- Bundlings (except xb and xb_03) as proposed by ADAS team

Material transport of W from walls

Result from full-W simulations: Transfer of W material from HFS belt limiter and outer limiter to divertors (mostly inner)





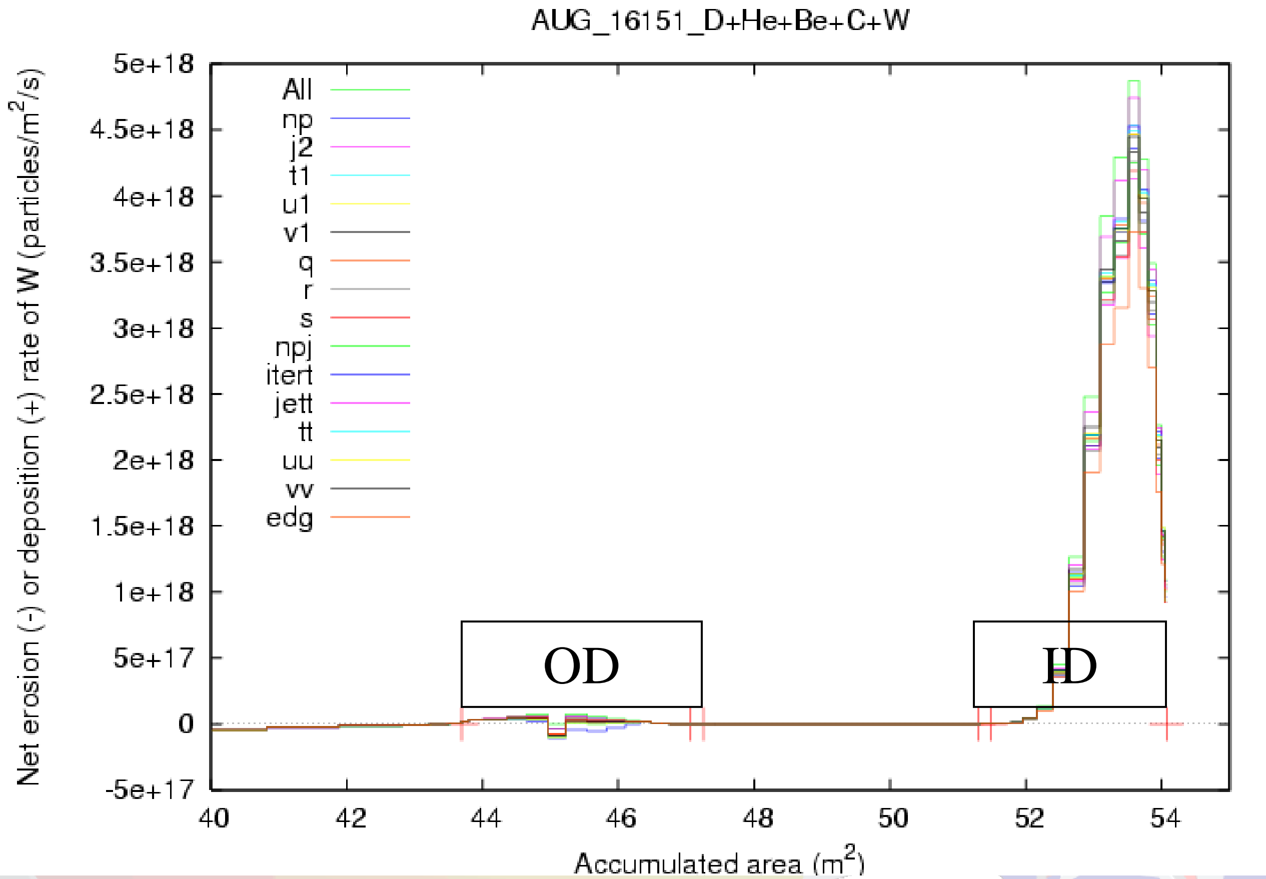
ID : Inner divertor
OD : Outer divertor

Bonnin

Outline colours = W net erosion/deposition in monolayers/second

What approximation does bundling introduce?
Case of material migration to the divertors

Bonnin



- Most bundling schemes underestimate net W deposition in ID by 5-20%
- 'jett' scheme most closely approximates full treatment (24 species with emphasis on lower ionization stages)
- 'itert' is only scheme to see wide net erosion zone in OD: also only to bundle together all lower ionization stages of W
- 'xb' and 'xb_03' to test how much detail of lower stages is necessary

SOLPS-B2.6: Adaptive scrape-off layer simulations

Extension of the B2 plasma fluid code (part of the SOLPS package)

- Moving to unstructured field-aligned anisotropic grids
- Enable solution-driven grid adaptation at runtime
- Extensive modernization of the B2 code base (towards multigrid, parallelization)
- Two new alternative adaptive solvers for B2:
  - B2.6-structured: hybrid FVM, structured grids
  - B2.6-unstructured: new high-resolution FVM, unstructured grids

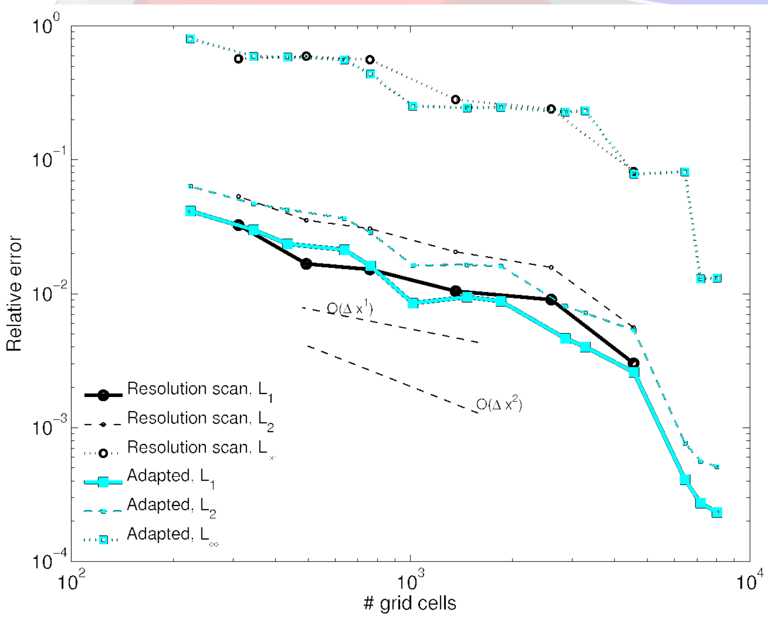
	B2.5	B2.6-structured	B2.6-unstructured
Hybrid FVM	✓	✓	-
High-resolution FVM	-	●	●
Grid adaptation	-	✓(structured)	✓(unstructured)
Standard physics model	✓	✓	●
Drift physics model	✓	✕	✕

Implementation status of the B2 code family. ✕ = not started, ● = partially completed, ✓ = completed, - = not possible with this version.

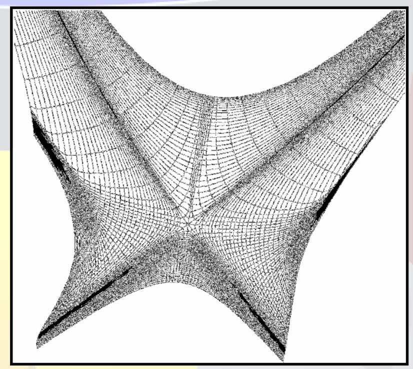
Klingshirn

B2.6-Structured: structured grid adaptation

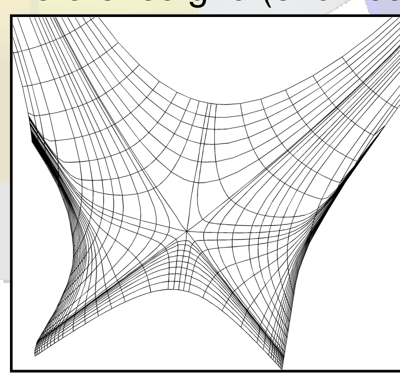
- Alternative solver for B2 with adaptive structured grids
- Comprehensive physics model maintained
- Exact backward compatibility to B2.5 ensured by extensive automated regression testing

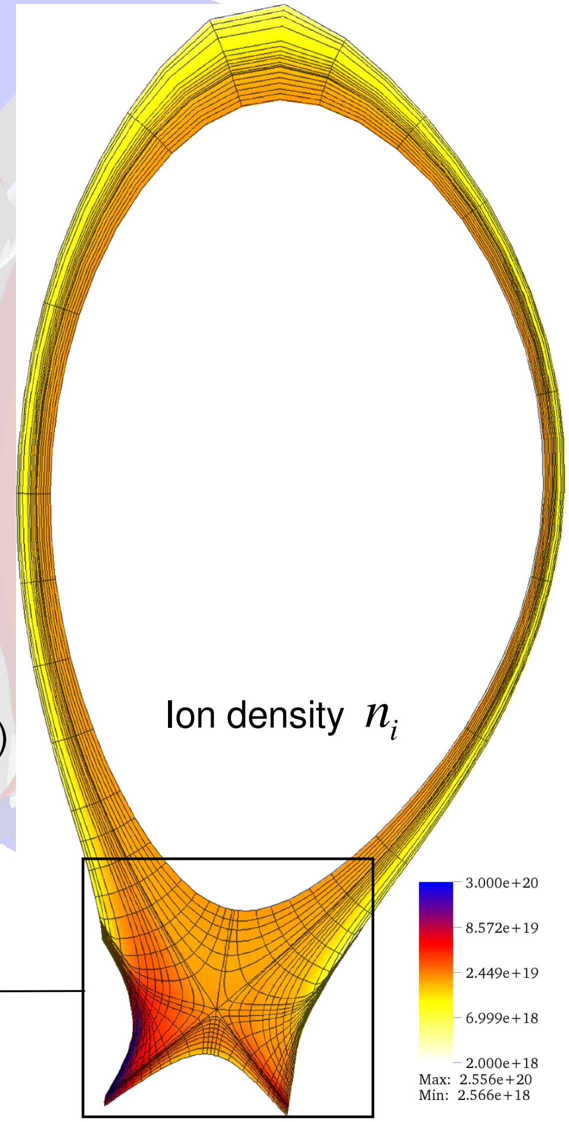


Relative ion density n_i error vs. grid cell count



Reference grid (8192 cells)





Adapted grid (1476 cells)

Klingshirn

B2.6-unstructured: fully unstructured grids

ASDEX Upgrade

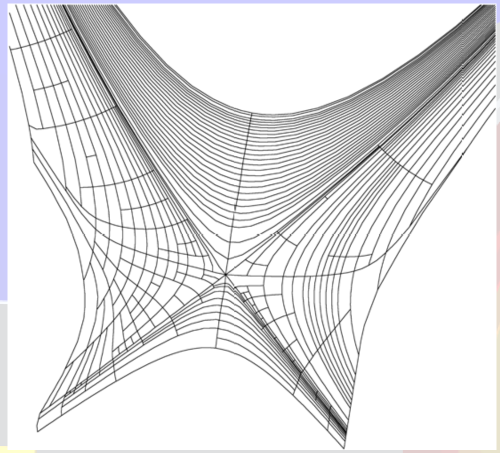
IPP

Central advances:

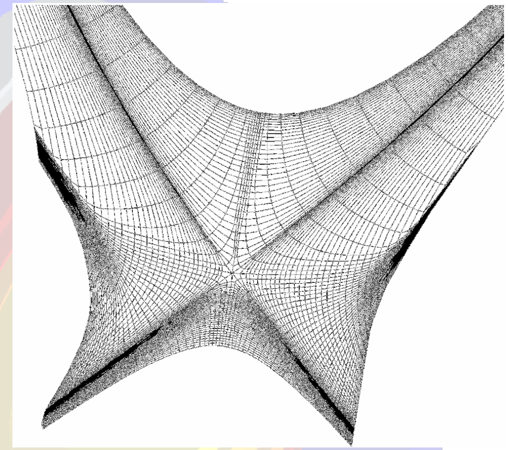
- Efficient global criteria-driven grid refinement and coarsening algorithms
- High-resolution FVM for complicated geometries

Current Status:

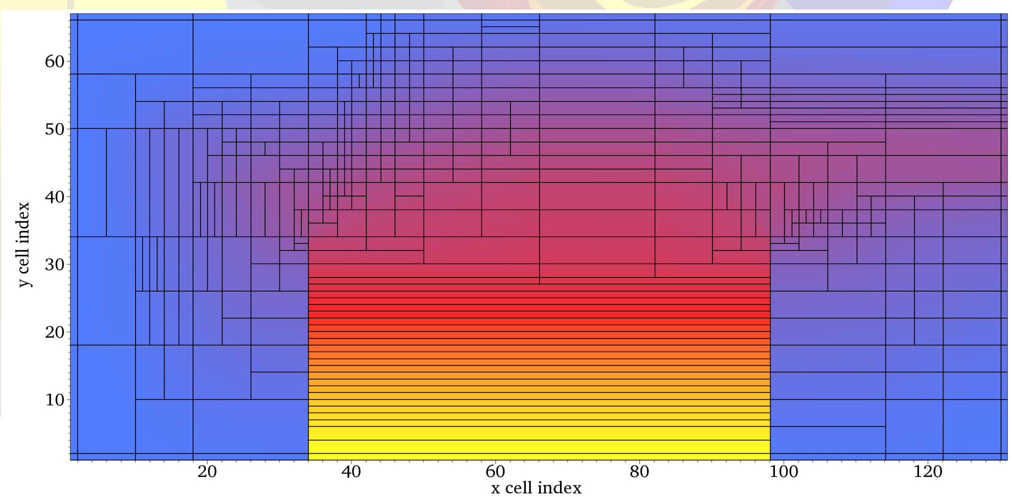
- New core advection-diffusion solver successfully verified on unstructured grids
- Grid adaptation algorithms completed
- Physics model implementation and testing ongoing



Solution-adapted grid (divertor plot, physical space)



Reference base grid



Full grid (computational space) with reference T_e solution

Klingshirn

ASDEX Upgrade

Problems in B2SOLPS5.0 with drifts

In spite of many simulations performed for L-mode shots, the old version has following problems:

1. **Small time step is required for L-mode.**
2. **Absence of convergence for H-mode.**
3. **Big radial convective fluxes in the core and small transport coefficients results in artificial numerical transport, which might change profiles. Especially pronounced inside the transport barrier.**

➔ **The code should be rewritten to avoid big radial convective fluxes.**

St Petersburg

Transformation of the equation system

The main idea is to replace large radial grad B driven convective fluxes by parallel fluxes with the same divergence both in particle and energy balance equations

St Petersburg

- **Old particle balance**

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{\sqrt{g}}{h_x}\frac{n_a T_i B_z}{Z_a e}\frac{\partial}{h_y \partial y}\left(\frac{1}{B^2}\right)\right)-\frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{\sqrt{g}}{h_y}\frac{n_a T_i B_z}{Z_a e}\frac{\partial}{h_x \partial x}\left(\frac{1}{B^2}\right)\right)=-\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{\sqrt{g}}{h_x}\frac{B_z}{Z_a e}\frac{\partial n_a T_i}{h_y \partial y}\left(\frac{1}{B^2}-\frac{1}{<B^2>}\right)\right)+\frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{\sqrt{g}}{h_y}\frac{h_z B_z}{Z_a e}\frac{\partial n_a T_i}{h_x \partial x}\left(\frac{1}{B^2}-\frac{1}{<B^2>}\right)\right)$$

- **New particle flux**

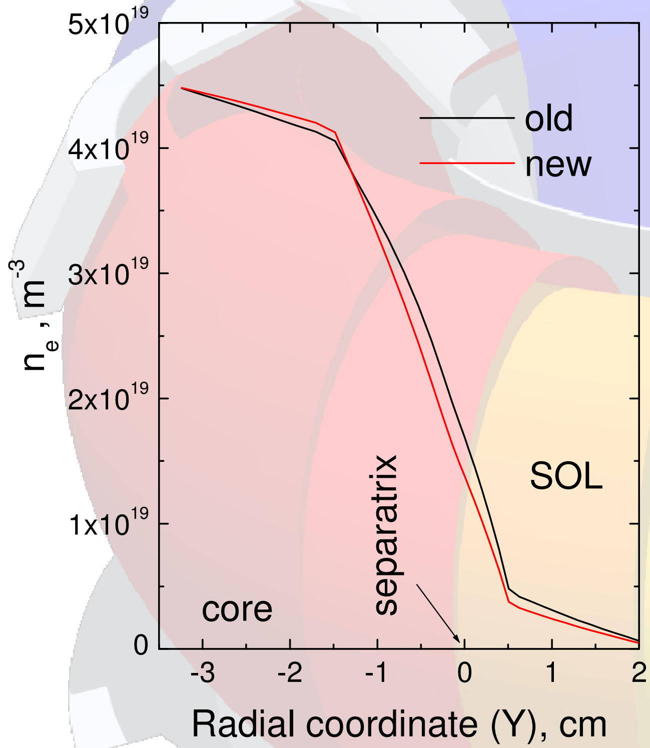
$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{\sqrt{g}}{h_x}n_a\left(b_x V_{\parallel}^{NEW}+b_z V_{\perp}^{(a)}\right)\right)+\frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{\sqrt{g}}{h_y}n_a V_y^{(a)}\right)=S^n-\frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{\sqrt{g}}{h_y}\frac{h_z B_z}{Z_a e}\frac{\partial n_a T_i}{h_x \partial x}\left(\frac{1}{B^2}-\frac{1}{<B^2>}\right)\right)$$

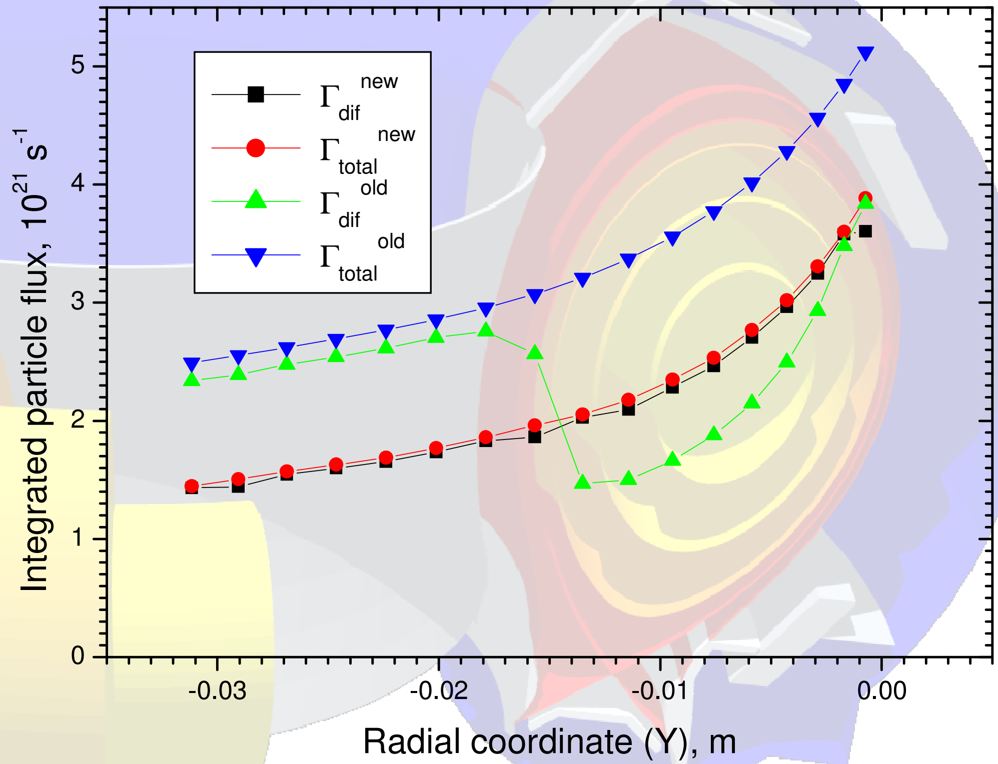
$$V_{\parallel}^{NEW}=V_{\parallel}-V_{\parallel}^{P.S.} \qquad V_{\parallel}^{P.S.}=\frac{B_z}{B_x B}\frac{1}{Z_a e n_a}\frac{\partial n_a T_i}{h_y \partial y}\left(1-\frac{B^2}{<B^2>}\right)$$

- **Heat fluxes were rewritten in the same way**

ASDEX Upgrade

H-mode simulations





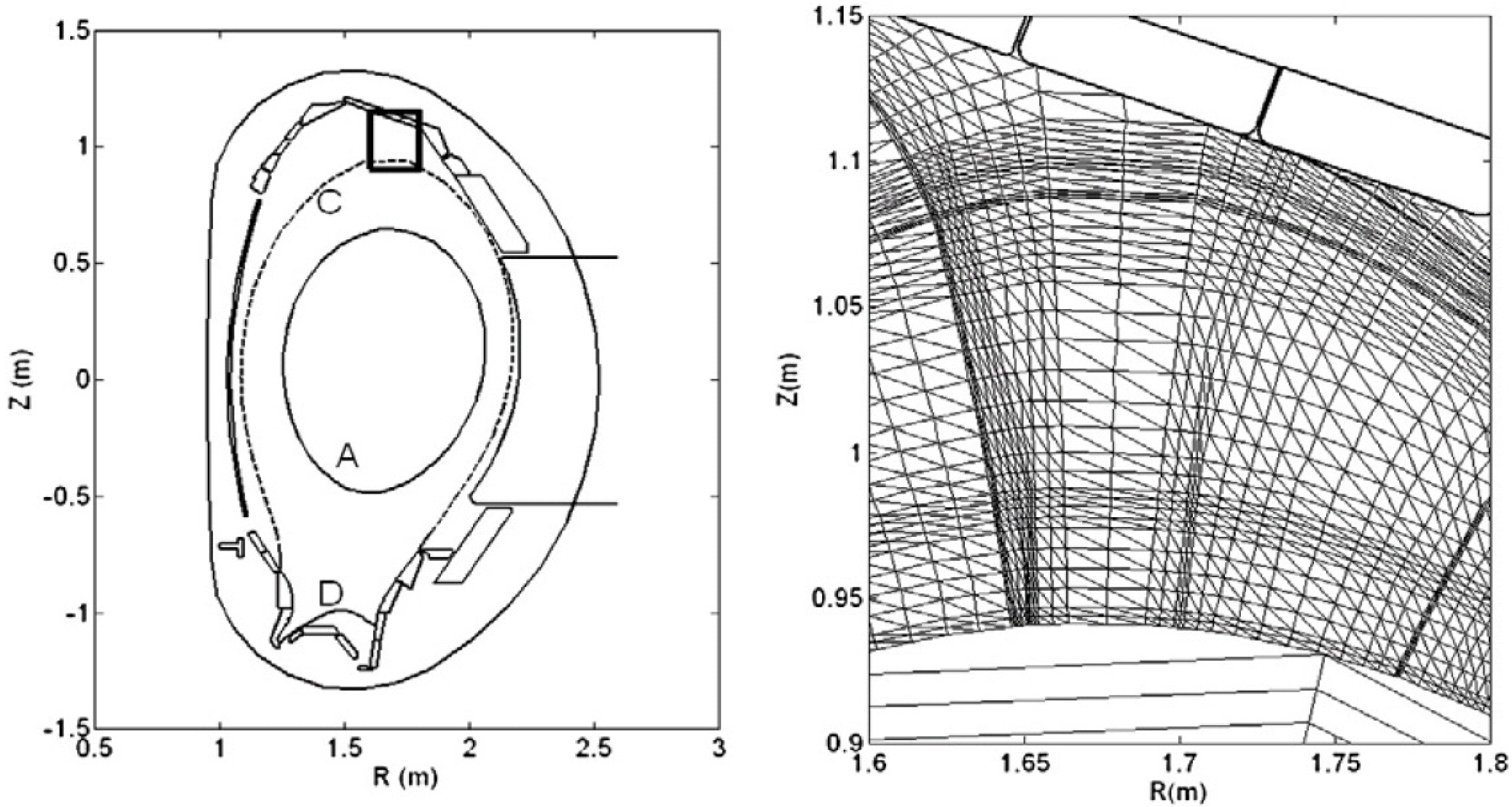
St Petersburg

Geometry extensions

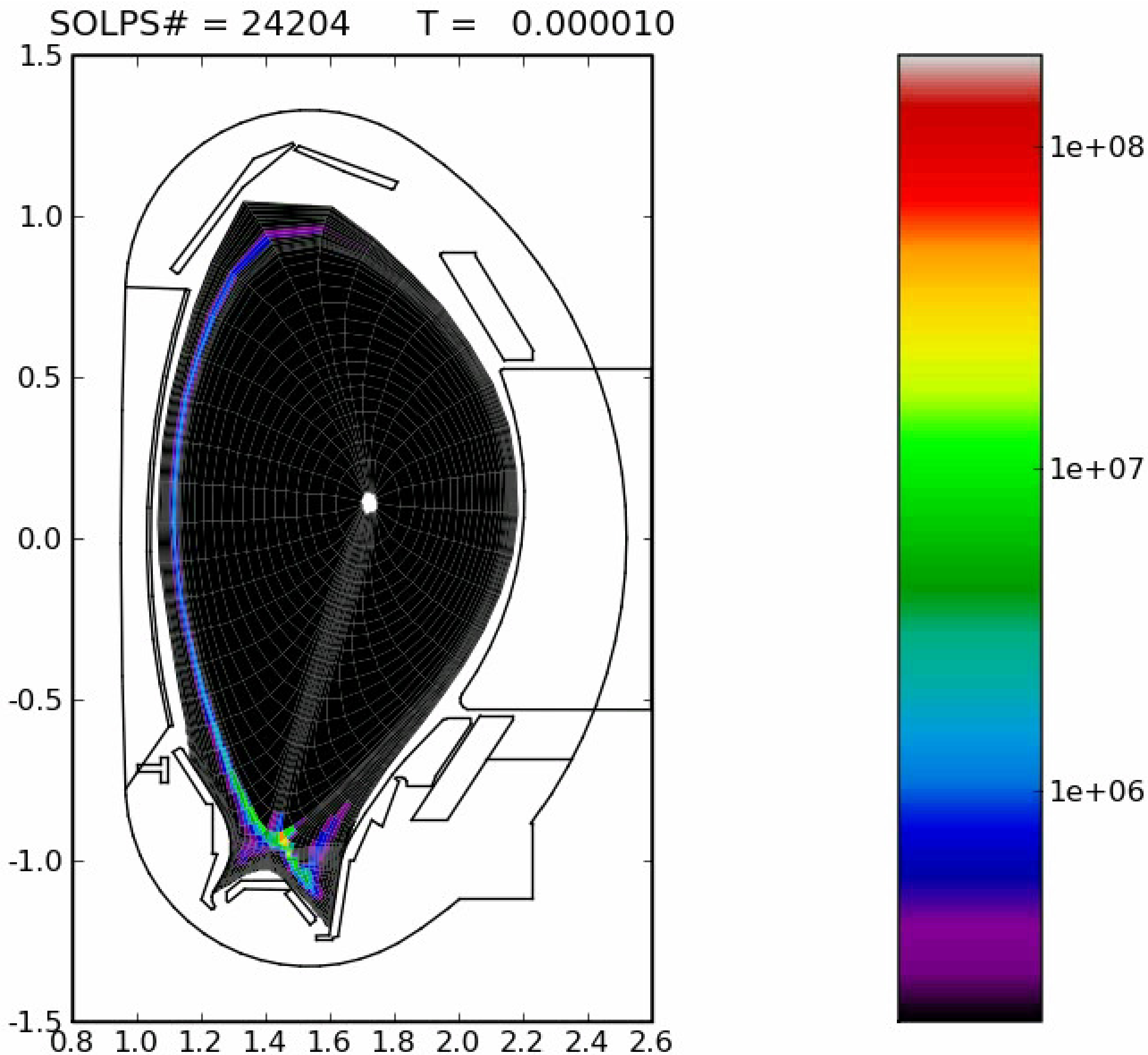
- Extensions to the real wall
  - Extension of the SOLPS grid
  - Use of the improved trace ion module currently under development in EIRENE
  - Couple to additional code
    - ASPOEL
  - Move to 3D code
    - EMC3-EIRENE
- Extensions to the core
  - Mediated
    - where the edge codes are used to provide boundary conditions for the core codes on the basis of fitting coefficients to the results of a number of edge runs
  - Direct
    - where the edge and core codes are directly coupled (future ITM development)
  - Avoided
    - where edge code is extended all the way to the centre of the plasma

Geometry extensions

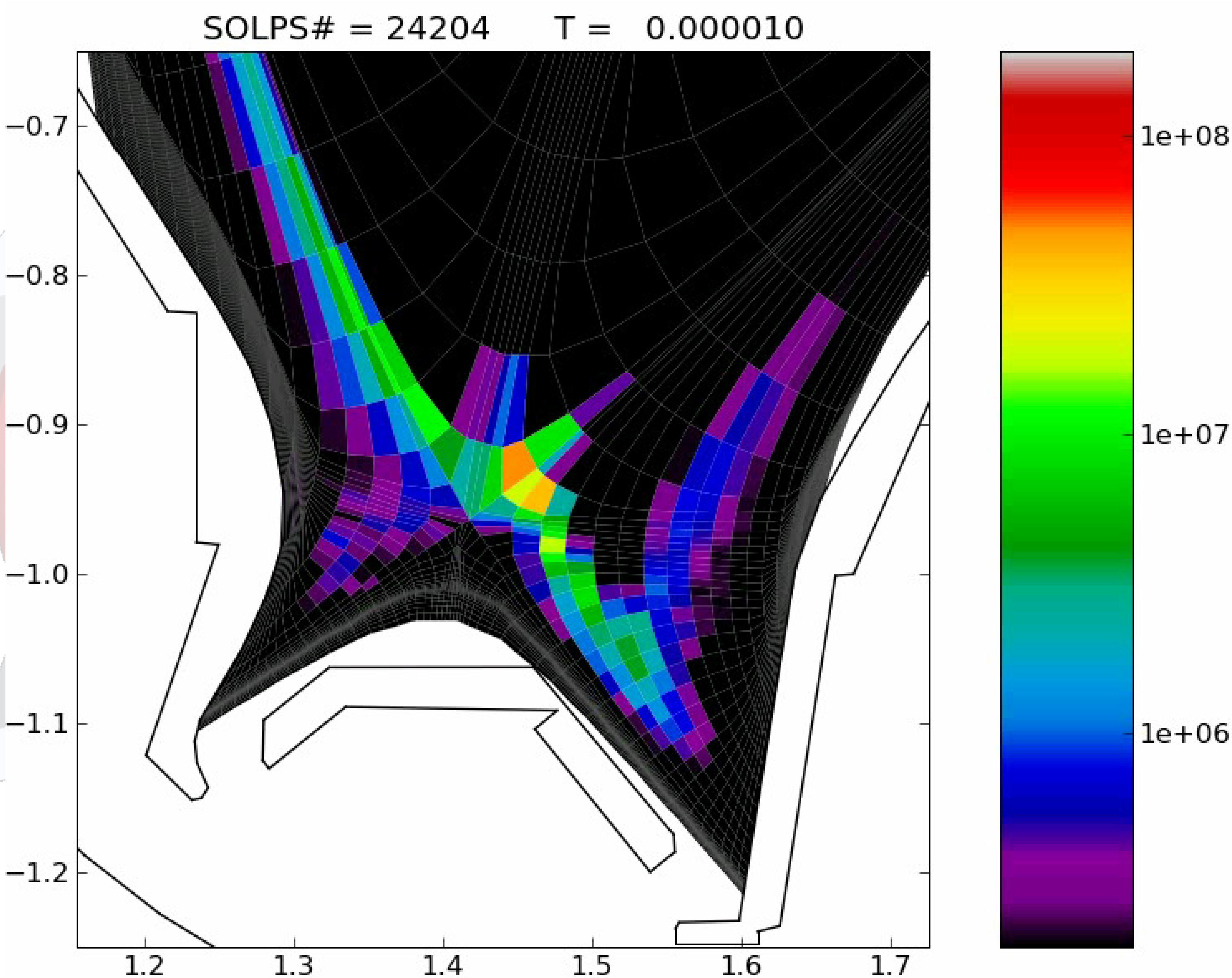
F. Subba et al. / Computer Physics Communications 179 (2008) 194–198



Geometry extensions



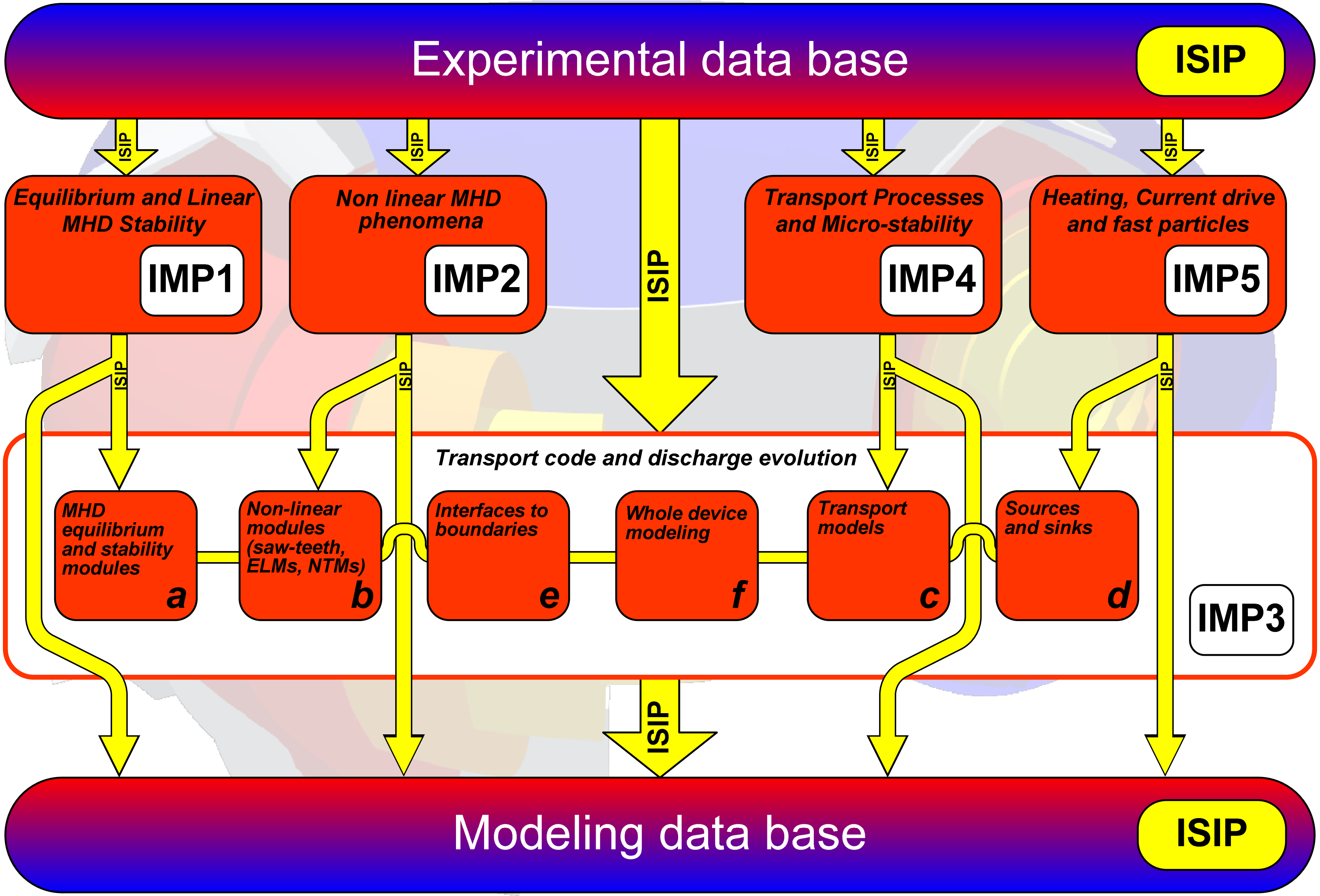
Geometry extensions



EFDA-ITM: CPOs, AMNS

- EFDA Task Force on Integrated Modelling is developing a framework for coupling codes
  - Kepler as work flow engine
  - CPOs for data
  - UAL to transfer and store data

ITM Structure

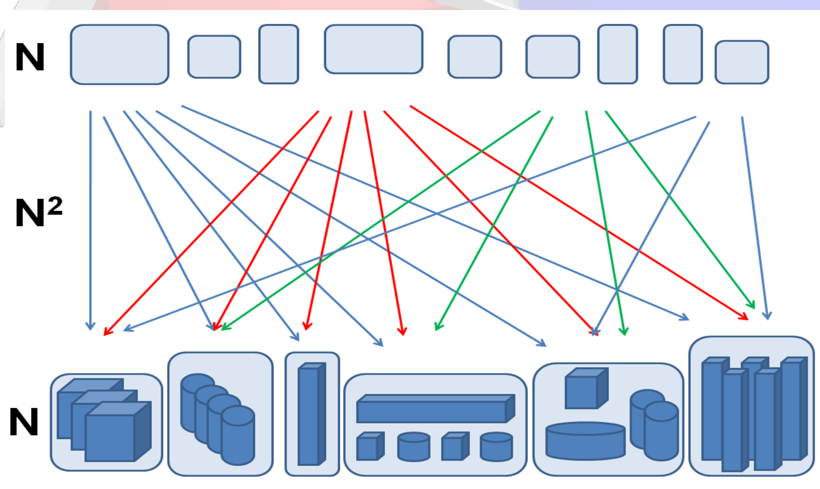


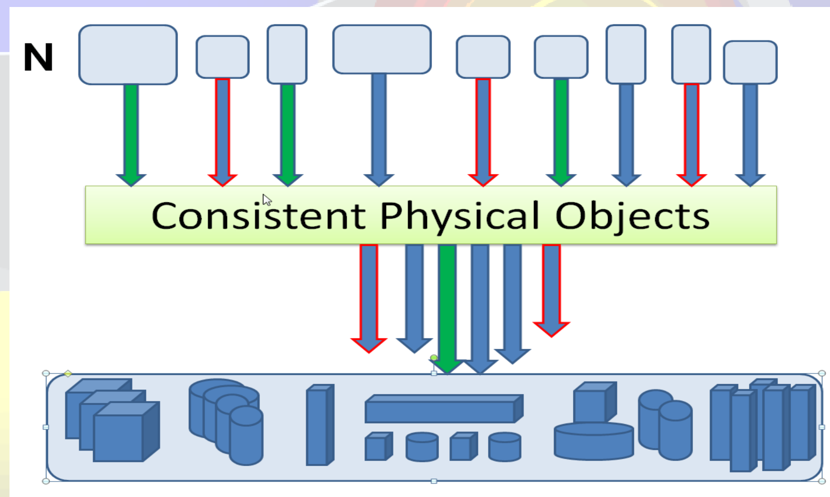
Kalupin, 2008

Coupling codes and applications

N modules integrated in N different applications

N modules coupled into a dynamic application framework



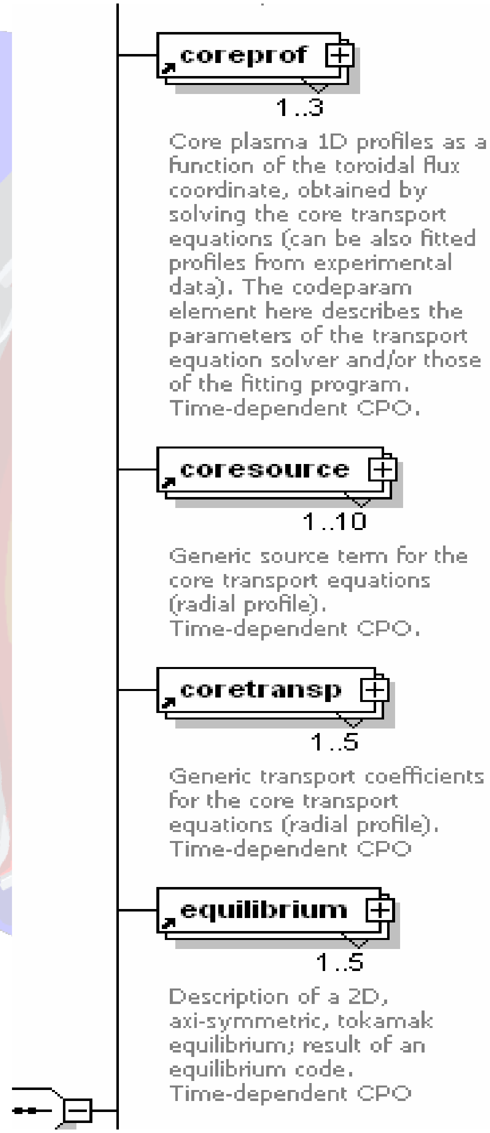


The data model – or ontology - is the key to providing a consistent framework!

Strand, ITM General Meeting 2009
Bastardised from David De Roure

What is a CPO?

- Consistent Physical Object
  - Data structure describing a piece of physics
    - From the experiment
    - From a code
  - Minimal data object to be passed to another code, or written to storage
- Input/Output using the UAL (Universal Access Layer)
  - Bindings for Fortran, C++, Matlab, Python
- Currently developing CPOs for edge
  - Spent a long time developing a general concept for storing data on grids



On the use of Atomic, Molecular, Surface and Nuclear (AMNS) data in the ITM-TF

- Version control of data imported to the ITM-TF data base is mandatory.
- The provenance of the data must be accurate and stored in the ITM database
- For "production" runs with ITM-TF codes using AMNS data it is important that the data have been given a stamp of approval by an expert.
- The AMNS data must be communicated to ITM-TF codes via a standardised interface (this should also ensure coherence between different ITM-TF codes needing the same type of data)

Accessing the AMNS data

Physics code

- Access to AMNS data only via interface
  - initialization (2)
  - finalization (2)
  - querying parameters (2)
  - setting parameters (2)
  - **getting data** (1)
- Separation between use of the data and the implementation of the data
- Code author doesn't need to become an expert in AMNS
- Ensures compatibility between codes

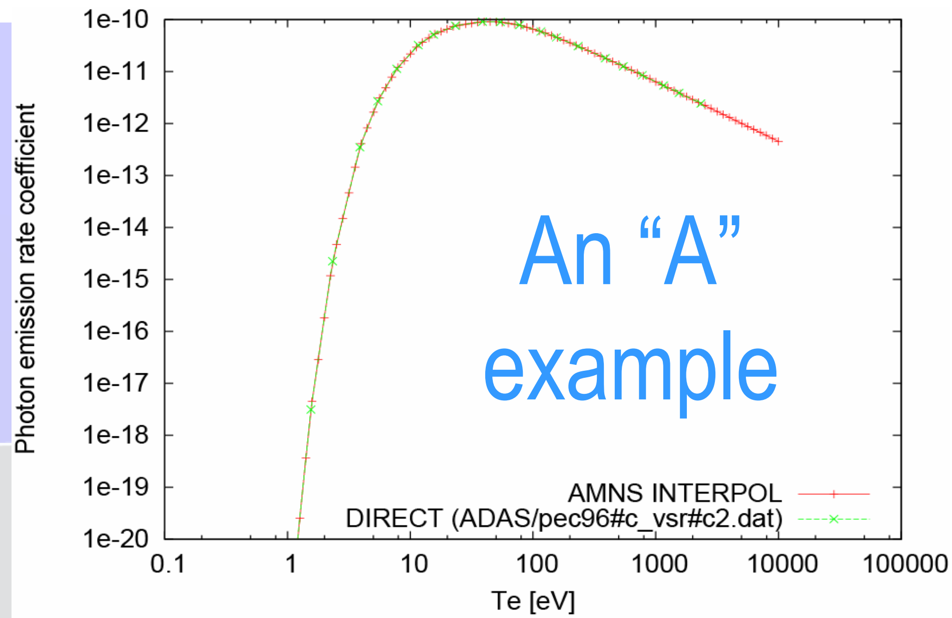
AMNS implementation

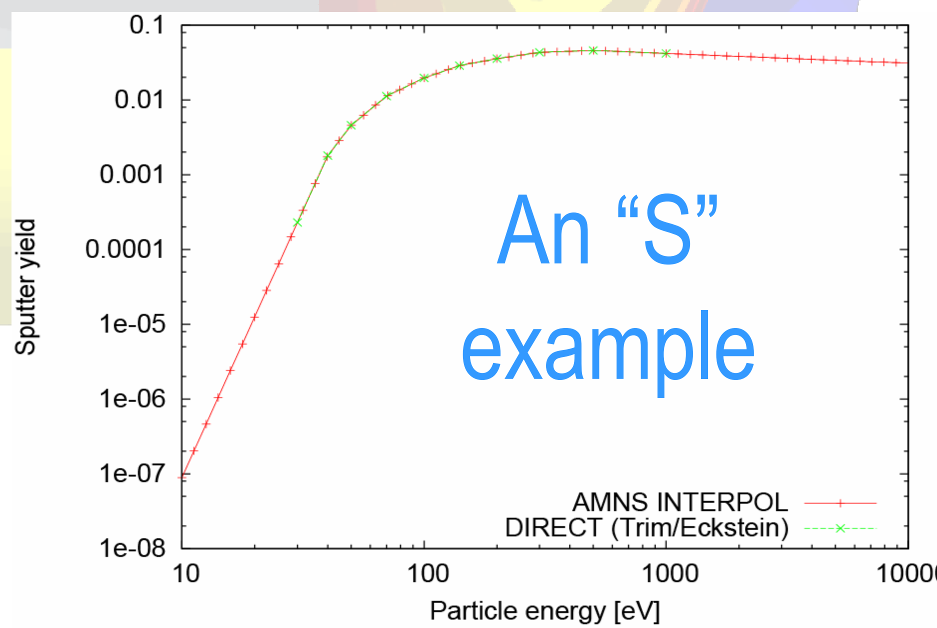
- Only accessed by a set of defined calls
- Implementation by AMNS experts
- Different versions can be supported
- Different implementations possible
  - Analytic formulae
  - Table lookup
- "Old" versions should always be recoverable (even if wrong)
- Should become easier to implement "new" data

Prototype example: AMNS

- A prototype has been implemented
  - As a F90 module using derived types
  - **Interface will handle error estimates in the AMNS data!**

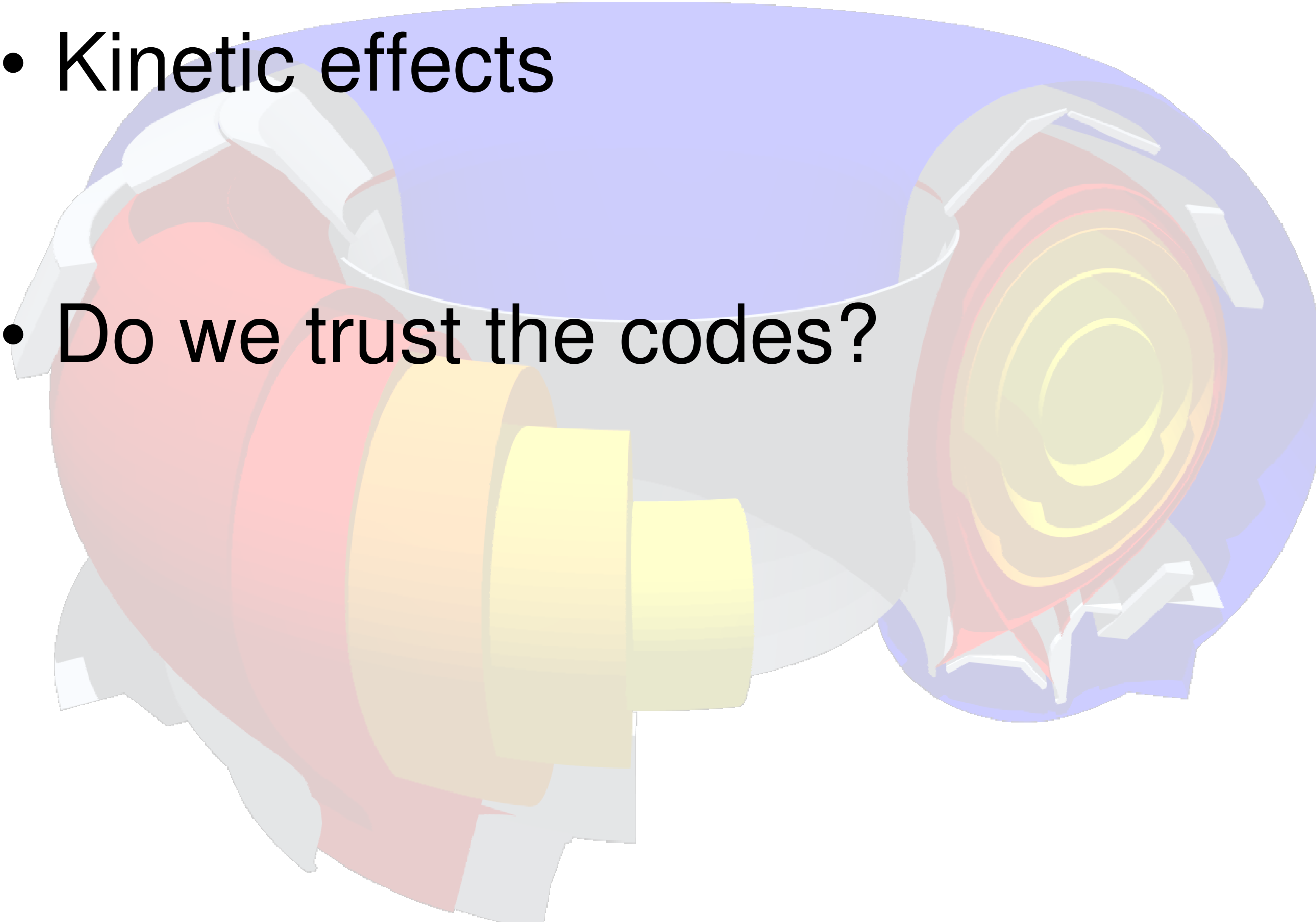
```
call ITM_AMNS_SETUP(amns)
query%string='version'
call ITM_AMNS_QUERY(amns,query,answer)
...
call ITM_AMNS_SETUP_TABLE(amns, lr_rx,
    species_lr, amns_lr)
query%string='source'
call
    ITM_AMNS_QUERY_TABLE(amns_lr,query,ans
    wer)
...
set%string='nowarn'
call ITM_AMNS_SET_TABLE(amns_lr,set)
...
call
    ITM_AMNS_RX(amns_lr,rate(:,:,0),ne,te)
...
call ITM_AMNS_FINISH_TABLE(amns_lr))
call ITM_AMNS_FINISH(amns)
```





Missing physics, V&V

- Kinetic effects
- Do we trust the codes?

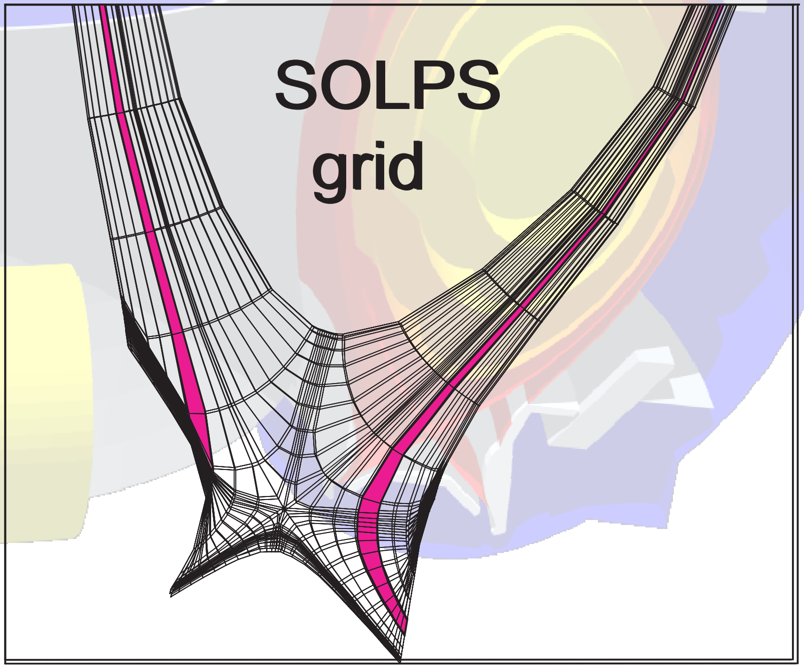


Basic version of kinetic plasma module for SOLPS

Chankin

- **Parallel electron kinetics.** Emphasis on parallel heat flux $q_{e||}$.
  Justification: $\chi_{e||} >> \chi_{i||}$. Fluid equations for ions (kinetic – later).
- **Perpendicular (radial) transport:** standard B2 treatment using *ad hoc* transport coefficients $\chi_{e\perp}$, $\chi_{i\perp}$, $D_{\perp}$, viscosity etc. (drifts – later; but No ion orbits ! (2D effect)).
- **1D+ structure.** Solves along field lines, then exchange (heat, particle) between flux surfaces
- Continuum **Fokker-Planck equation, 1D2V** ($v_{||}$,$v_{\perp}$)
- **Plasma quasi-neutrality** assumed, electron equilibrium along **B**, Debye sheath not resolved, "logical sheath condition" at divertor targets
- **Grid resolution:** as in SOLPS or better
- **Interactions with neutrals and impurities:**

  handled by SOLPS (Eirene and B2)



Progress

- Fokker-Planck equation for electron distribution function can now be solved
  - with full non-linear collision operator for electron-electron collisions
- Solutions (on the 200x400 grid, in parallel and perpendicular velocity coordinates) are quite precise,
  - to be able to correctly describe energetic electrons from the tail of the Maxwellian distribution that are mainly responsible for parallel electron heat conduction.
- Another part of the future code is to describe parallel electron propagation (along the field lines) and interaction with the target (effect of the Debye sheath).
  - This part has to be further developed, before the Fokker-Planck (Coulomb collision operator) can be coupled to it.

Chankin

Benchmarking of the 2D edge fluid codes

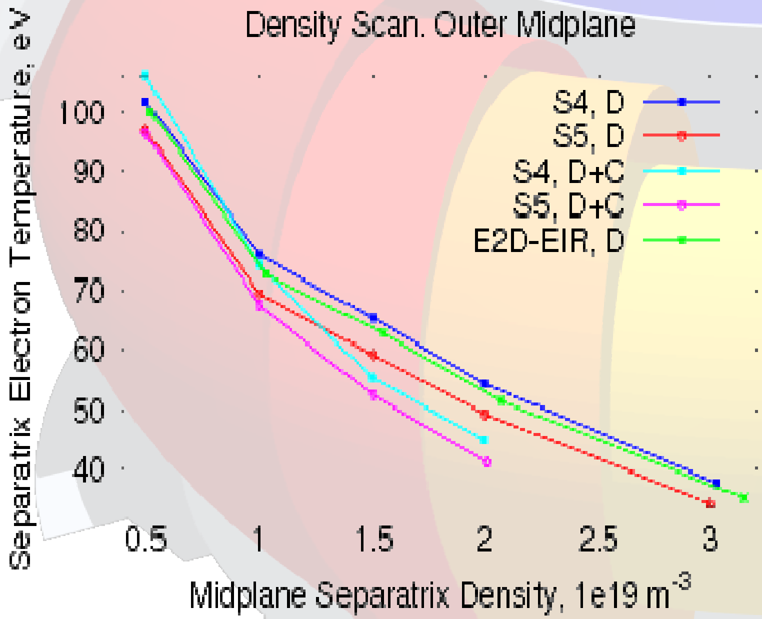
ASDEX Upgrade

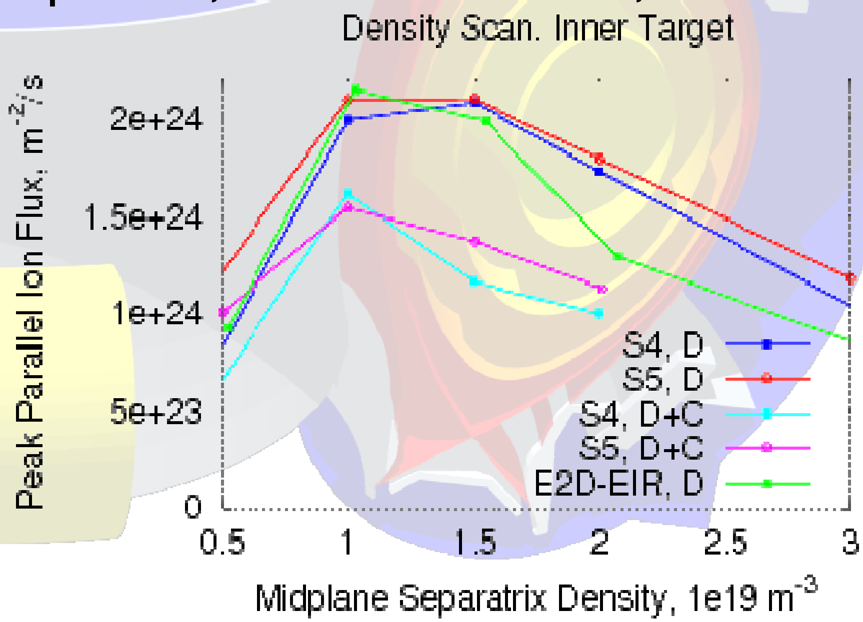
IPP

- V. Kotov (FZJ/ITER), D. Coster (IPP), S. Wiesen (FZJ/JET)
- SOLPS4.3 / SOLPS5.0 / EDGE2D-EIRENE

Kotov

JET #50401, 2.5 MW SOL input power, kinetic neutrals, w/o drifts





- Agreement within 15 % upstream (separatrix)
- Agreement within a factor of 2 at the targets

Importance of Detachment

- ITER designed to operate in the semidetached regime on the basis of SOLPS calculations
- simulation of detachment on present machines not always successful (Wischmeier et al, previous PSI and references therein)
- main problem seems to be the asymmetry in detachment between inner and outer target
- perform a study to see what affects this asymmetry
- use SOLPS5 code package
  - B2.5 fluid plasma code
  - EIRENE Monte-Carlo neutrals code (though some simulations used the B2.5 fluid neutrals model(

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Variations performed

- ✗ evolving (puffed) or steady state (feedback)
- ✗ vertical or horizontal target
- ✗ fluid or kinetic neutrals
- ✗ power scan
- ✗ effects of transport coefficients depending in upstream density
- ✗ D *vs* D+C
- ✗ with/without ELMs
- ✓ with/without hot electrons
- ✓ drifts

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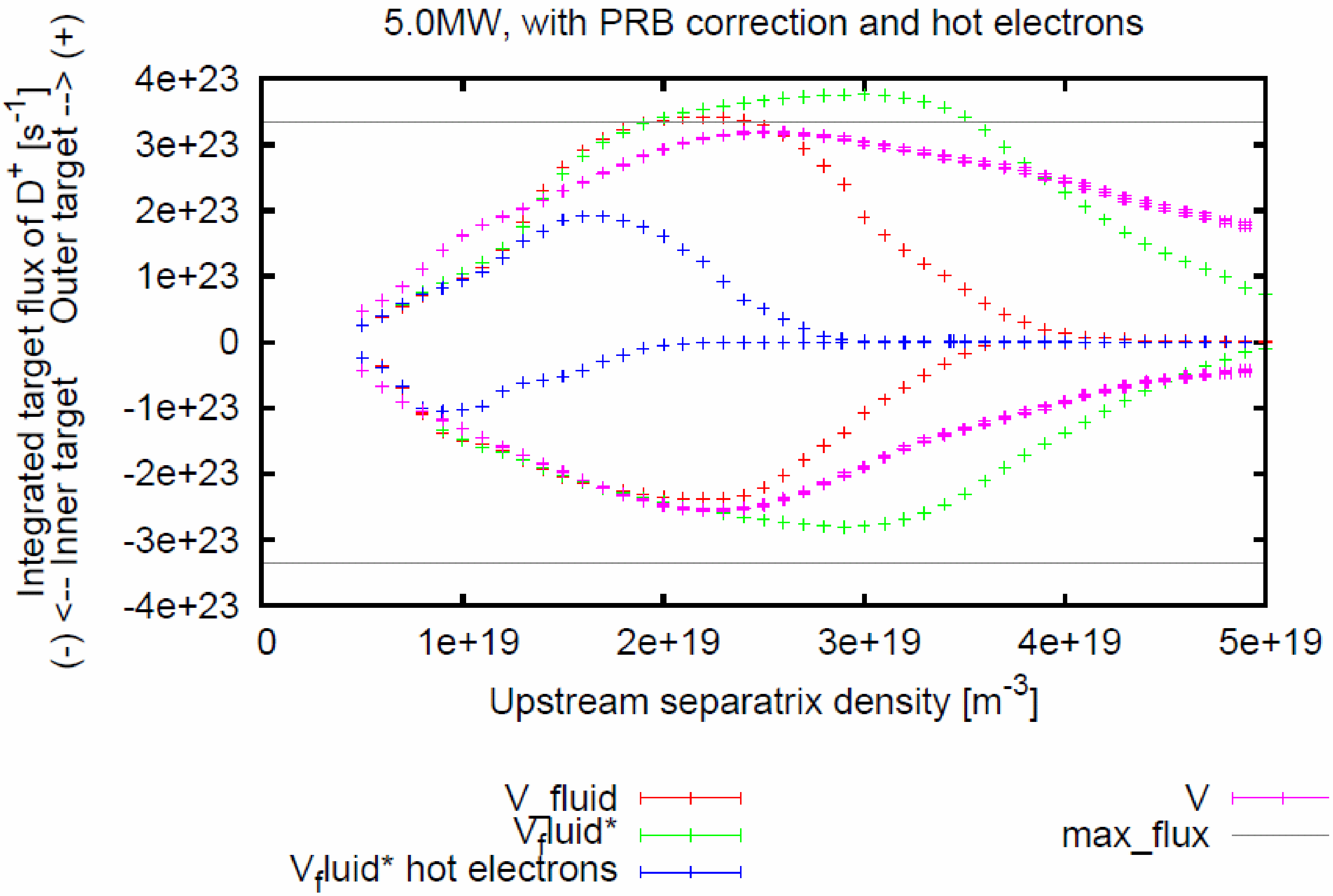
Hot electrons



Integral target fluxes for the 5.0MW cases.

Big effect on the rollover asymmetry

Lowers the rollover densities

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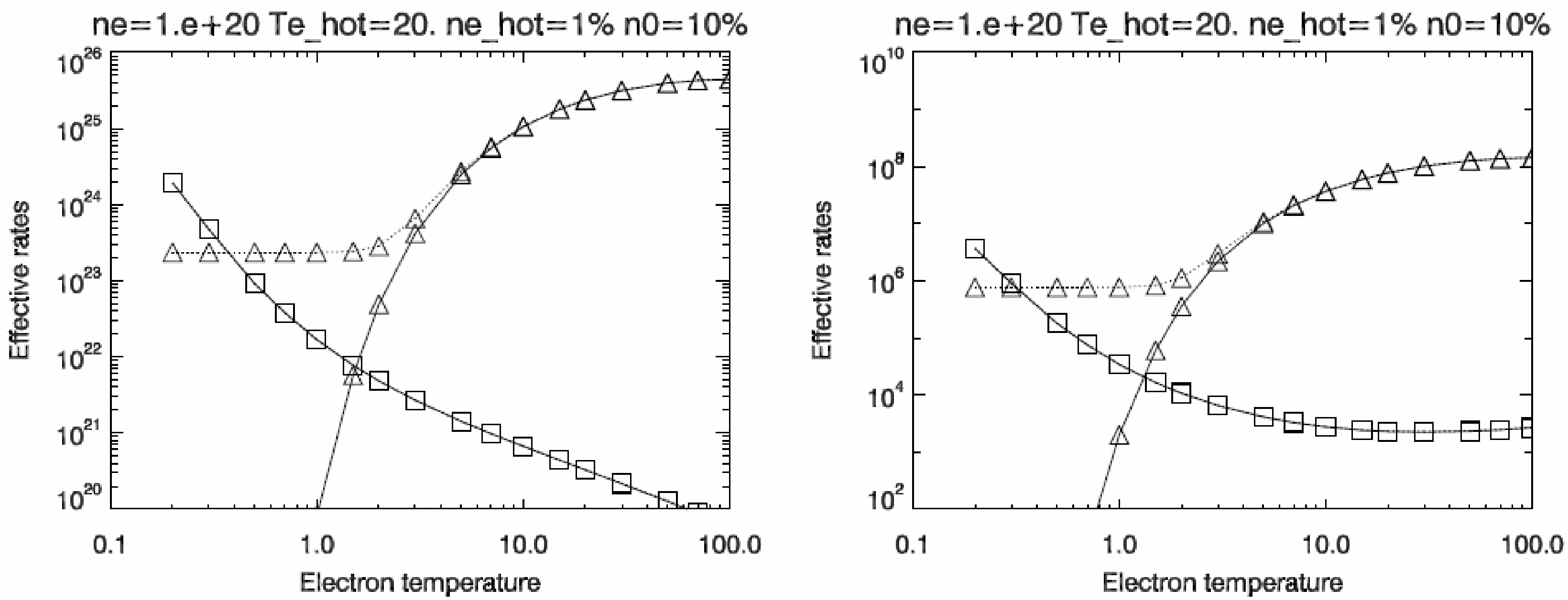
Hot electrons

99% of the atomic physics rates based on the local temperature and density

+

1% of the atomic physics rates based on 20 eV electrons and the local density



Rates for particles (l) and energy sources (r) for ionization (triangles) and recombination (squares). Dotted with the hot electrons, solid without.

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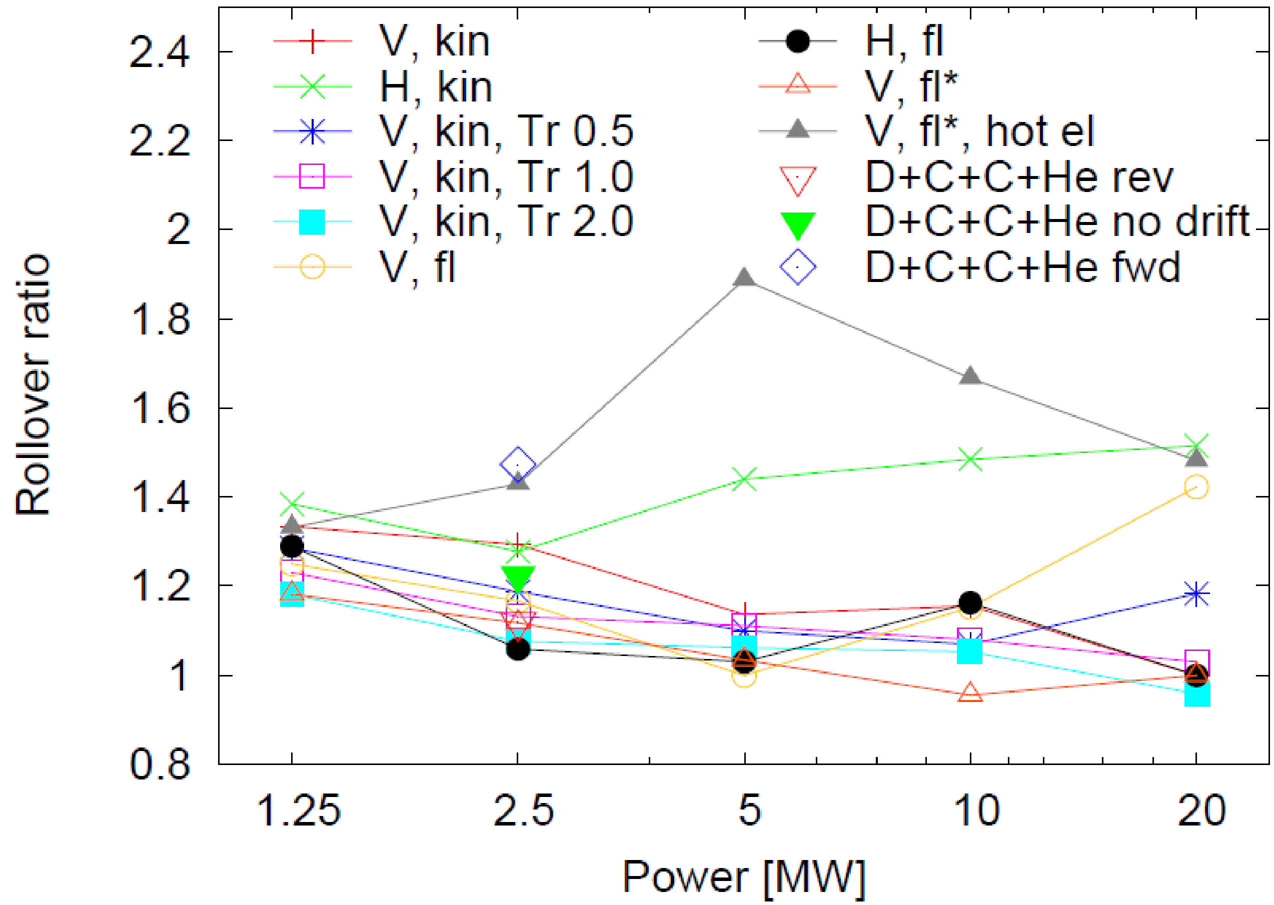
Detachment



Ratios of the roll-over fluxes.

Strongest effect from hot electrons
Weaker effect from drifts
Other effects even smaller

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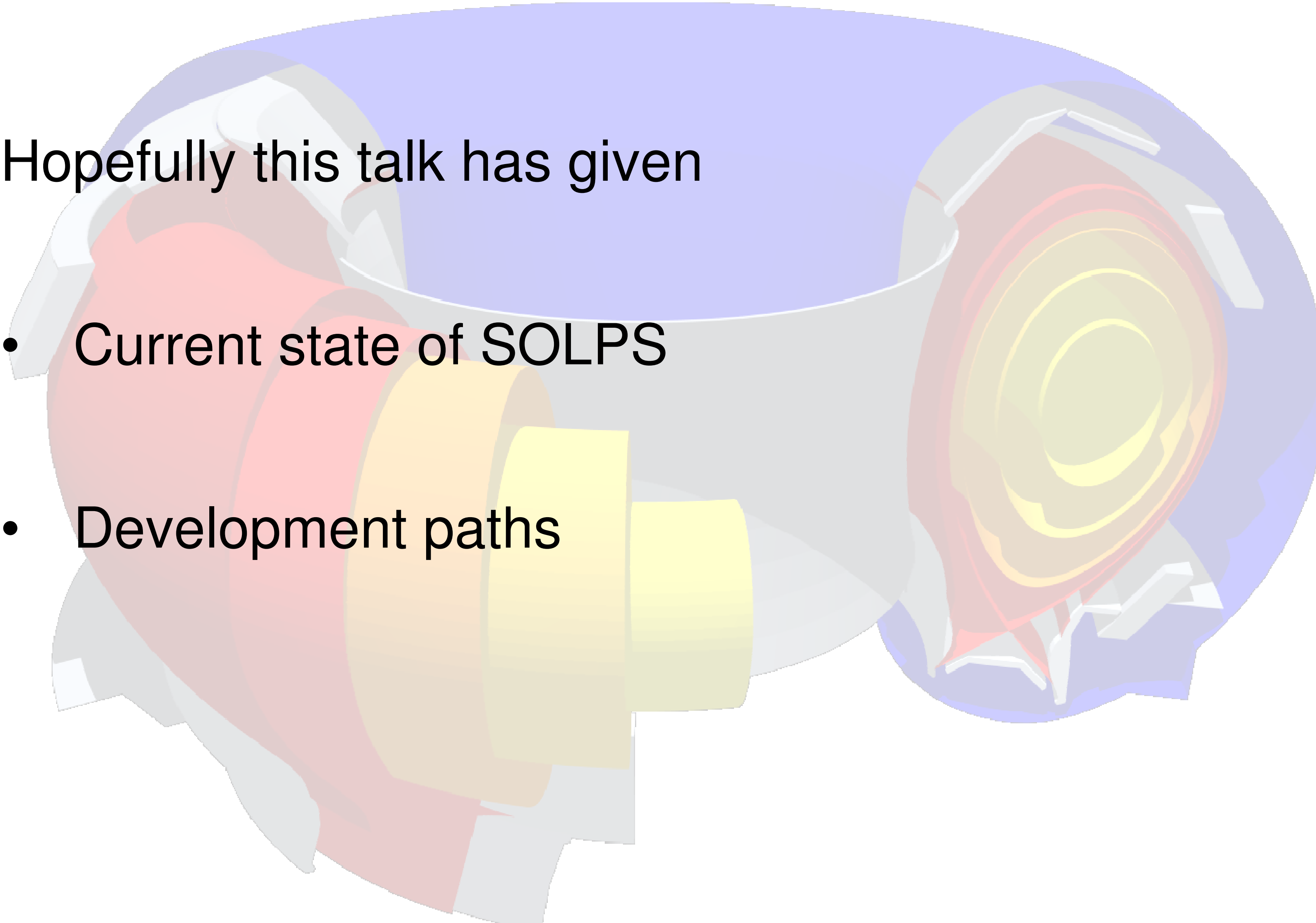
ASDEX Upgrade

Summary



Hopefully this talk has given

- Current state of SOLPS
- Development paths

Code/module requirements/status

Phase I (initial porting)

(A) porting to the ITM Gateway (runs on ITM Gateway, compilers, libraries, etc.)

(B) completion of “grant of software license and rights to the ITM-TF” procedure

(C) creation of a project under GForge and code under subversion (on the ITM Gateway or mirrored there)

Phase II (preparation of stand-alone module)

(D) conversion into a module using CPOs

(E) conversion of code specific input to XML

(F) creation of standalone wrapper for testing (“test bed”)

(G) provision of standard test cases

(H) standardized build procedure (make)

(I) standardized test procedure

Phase III (preparation of Kepler actor)

(J) creation of a Kepler actor

(K) creation of a Kepler test workflow

(L) benchmark of Kepler module against original version of code

(M) verification of Kepler module (code-code benchmarks)

Phase IV (documentation)

(N) code documentation (for developers and maintainers)

(O) user documentation (for users)

Phase V (release candidate cycle)

(P) validation by module author/responsible officer

(Q) release candidate for Kepler module (approved by Project Leader)

Phase VI (release cycle)

(R) validation by IMP

(S) release of Kepler module (approved by Task Force leader)