On recent massively parallelized PIC simulations of the SOL

D. Tskhakaya

Association EURATOM-ÖAW, University of Innsbruck, A-6020 Innsbruck, Austria

Andronikashvili Institute of Physics, 0177 Tbilisi, Georgia

Outline

- Motivation
- Description of the model
- Discussion of simulation results
- Boundary condition for the ion speed
- Conclusions

Do we need kinetic modelling of the SOL?

Full kinetic codes

- are too complex
- have low dimensionality
- (usually) are not user friendly
- simulations are fluctuative
- are CPU extensive

Yes we need

Why do we need kinetic SOL models

- Low collisionality of the SOL

$$\nu(V) = \left(\frac{V_T}{V}\right)^4 \nu^*, \quad \nu^* \sim 10^{16} \frac{L_\parallel n}{T^2}$$

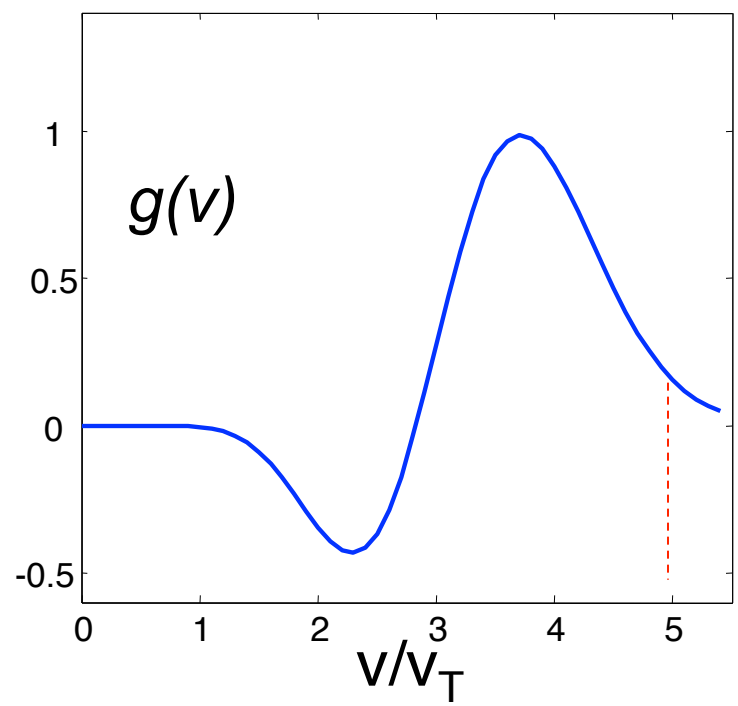
Energy flux: V_{max} ?

Kinetic equation for el. [Chodura CPP 1992)]

$$\mu V \frac{\partial}{\partial s} f_e - \frac{e}{m} E \frac{1-\mu^2}{V} \frac{\partial}{\partial \mu} f_e = C_{ei}, \quad I = 0$$

$$q_\parallel \sim \int g(V) dV$$

$$V_{\max} = 5V_T, \; \nu^* \approx 600$$



- Plasma sheath is a kinetic object

Assumptions usually made in derivation of fluid equations

- Interaction with impurity, neutrals and PSI are added to the fluid equations as particle, momentum and energy sources and sinks. The velocity distribution functions used for derivation of transport coefficients are not recalculated. Hence, it is assumed that the corresponding corrections are small.

$$\frac{\partial A}{\partial t} + \nabla \cdot \Gamma_A = S_{ources} - S_{inks}$$

- Ion shift velocity is smaller than the thermal one $V_i << V_T$.
- Fokker-Plank collision operators are simplified using $m_i/m_j << 1$

In general, none of these conditions is satisfied in the SOL!

Fokker-Plank codes

$$\left[\mathbf{V}\frac{\partial}{\partial \mathbf{r}} + \frac{e}{m}\left(\mathbf{E} + \mathbf{V}\times\mathbf{B}\right)\frac{\partial}{\partial \mathbf{V}}\right] f\left(\mathbf{r},\mathbf{V}\right) = C_{FP} + C_{BGK} + S$$

- Particle distribution function is calculated directly
- Relatively low numerical noise

- Low dimensionality, 1D3V, 2D2V
- Implementation of exact atomic and PSI processes is not trivial

Particle-in Cell (PIC)/ Monte Carlo (MC) codes

$$\frac{d\mathbf{V}_i}{dt} = \frac{e_i}{m_i}\left(\mathbf{E} + \mathbf{V}_i \times \mathbf{B}\right) + St$$

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_i,$$

- High dimensionality, up to 3D3V
- Parallelization is straightforward
- A&M and PSI processes can be implemented with relative easy

- Special care has to be taken to keep numerical fluctuations below some acceptable level

Scheme of the electrostatic PIC

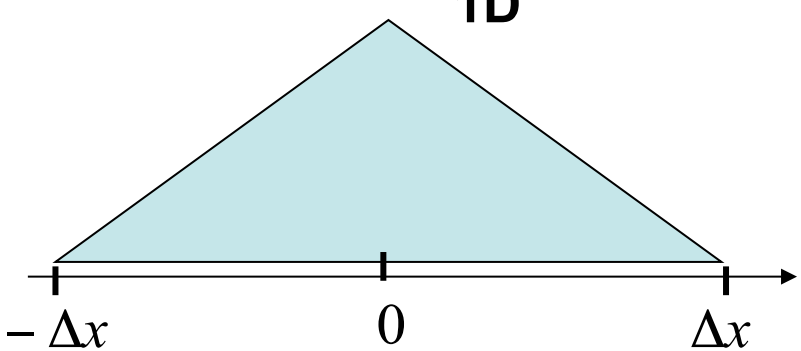
$$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_i, \quad k = 1,\ldots,N$$

$$\frac{d\mathbf{V}_i}{dt} = \frac{e_i}{m_i}\left(\mathbf{E} + \mathbf{V}_i \times \mathbf{B}\right) + MC$$

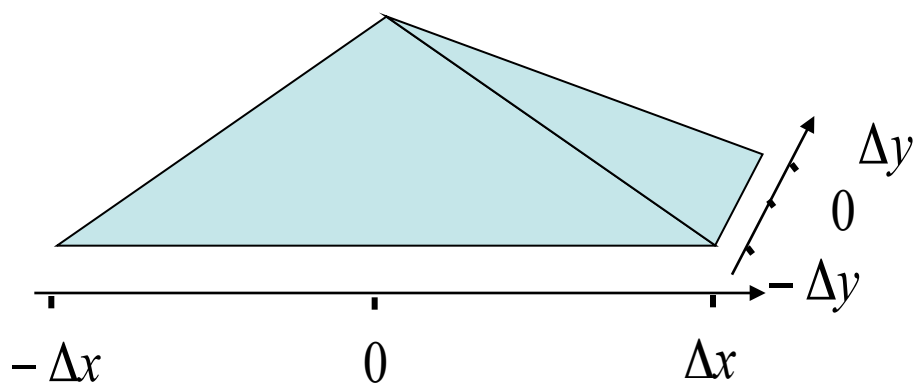
Statistical model for collisions and PSI

$$\nabla\mathbf{E}(\mathbf{r}) = -\frac{1}{\varepsilon_0}\sum_i e_i S(\mathbf{r},\mathbf{r}_i)$$

1D



2D



Some estimations

PIC requirements

$$\Delta t < \frac{1}{\omega_{pl}}$$

$$\Delta x \leq \lambda_D$$

$$N_{pc} > 100$$

SOL paralmeters ~

$$n \sim 10^{19}\ m^{-3}$$

$$T_e \sim 20\, eV$$

$$size \sim 15 \times 5 \times 0.01\ m$$

$$\Delta t \sim 2 \times 10^{-13}\ s$$

$$\lambda_D \sim 10^{-5}\, m$$

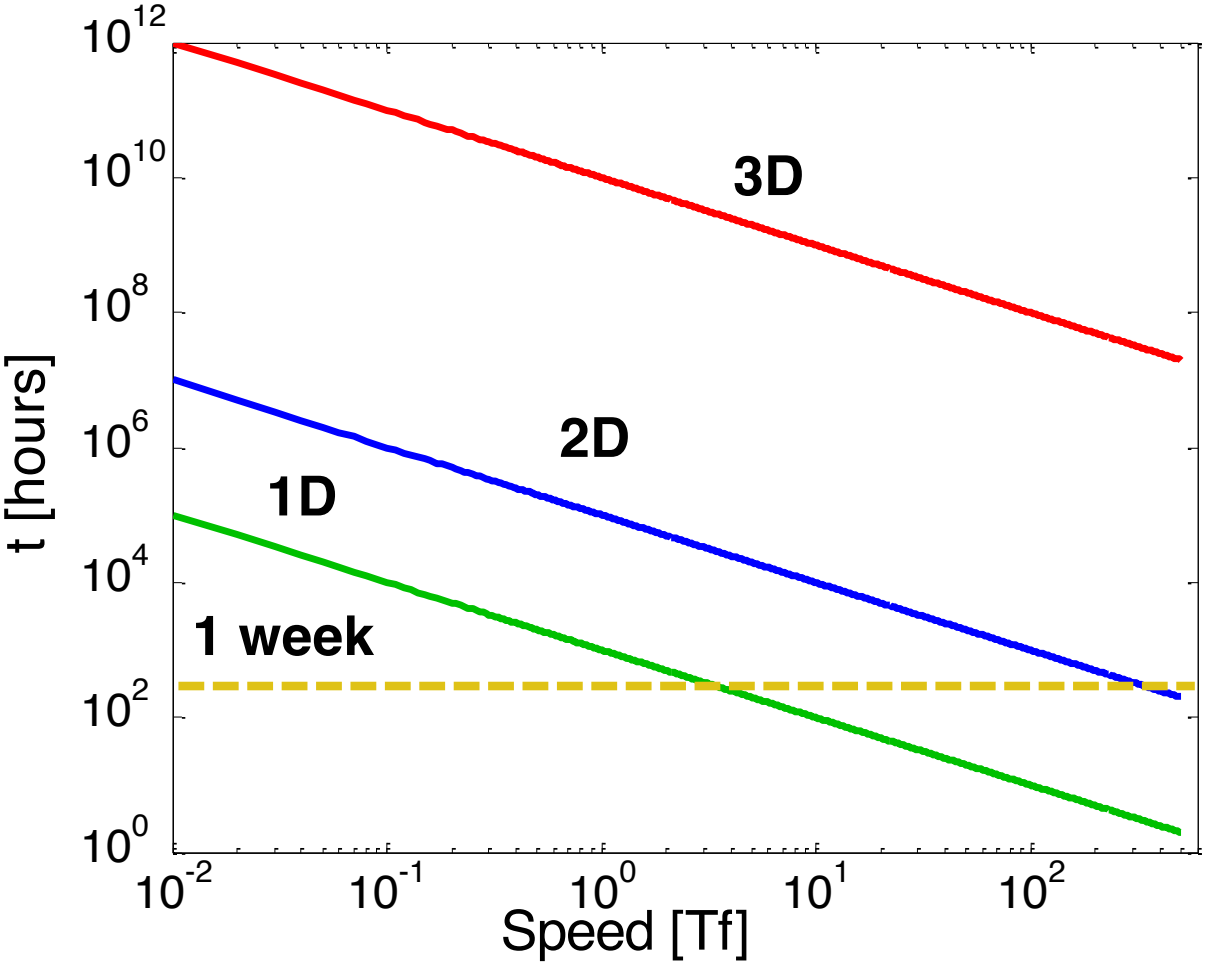
$$size \sim 1.5.10^6 \times 5.10^5 \times 10^3\ \lambda_D$$

$$N_p \sim 10^{15}$$

World record: $N_p \sim 10^{11}$

Can we do low dimensional models?

Some estimations (ii)



Real time required for plasma edge simulations vs. computer speed

$$t \sim N_{particle} \times N_{time\_steps} \times N_{fl.per\_step}$$

Tf = Tera flop, **flop** - floating Point Operations Per Second; The speed of fastest **PC** ~ **0.05 Tf**

Kinetic models of Scrape-off layer

1D SOL models

Procassini: NF 90, JNM 92

Chodura: CPP 88, ECA 90, CPP 92

Bergmann: PoP 94, NF 02

Igitkhanov (FP): CPP 93, 94, ECA 94

Takizuka: CPP 00, PoP 00, JNM 01, TFT 01

Batischev (FP): PoP 96, 97, 98

Pitts: NF 07

Gunn: PoP 07

Tskhakaya: CPP 08, JNM 09, 10

2D SOL models

Bergmann: CPP 96, 98, CzJP 98

Takizuka: JNM 03, CPP 10

Subba: CPP 02

Divertor plasma models

Brooks: PoP

Devaux (FP): PPCF 08

Tacogna: JNM 07, CPP 08

	N_{cell}	$N_{p/cell}$	$N_{species}$	M_i/m_e
Chod.:	200	<100	2	400
Rec.:	50 000	1000	>10	actual

Tskhakaya: CPP 08

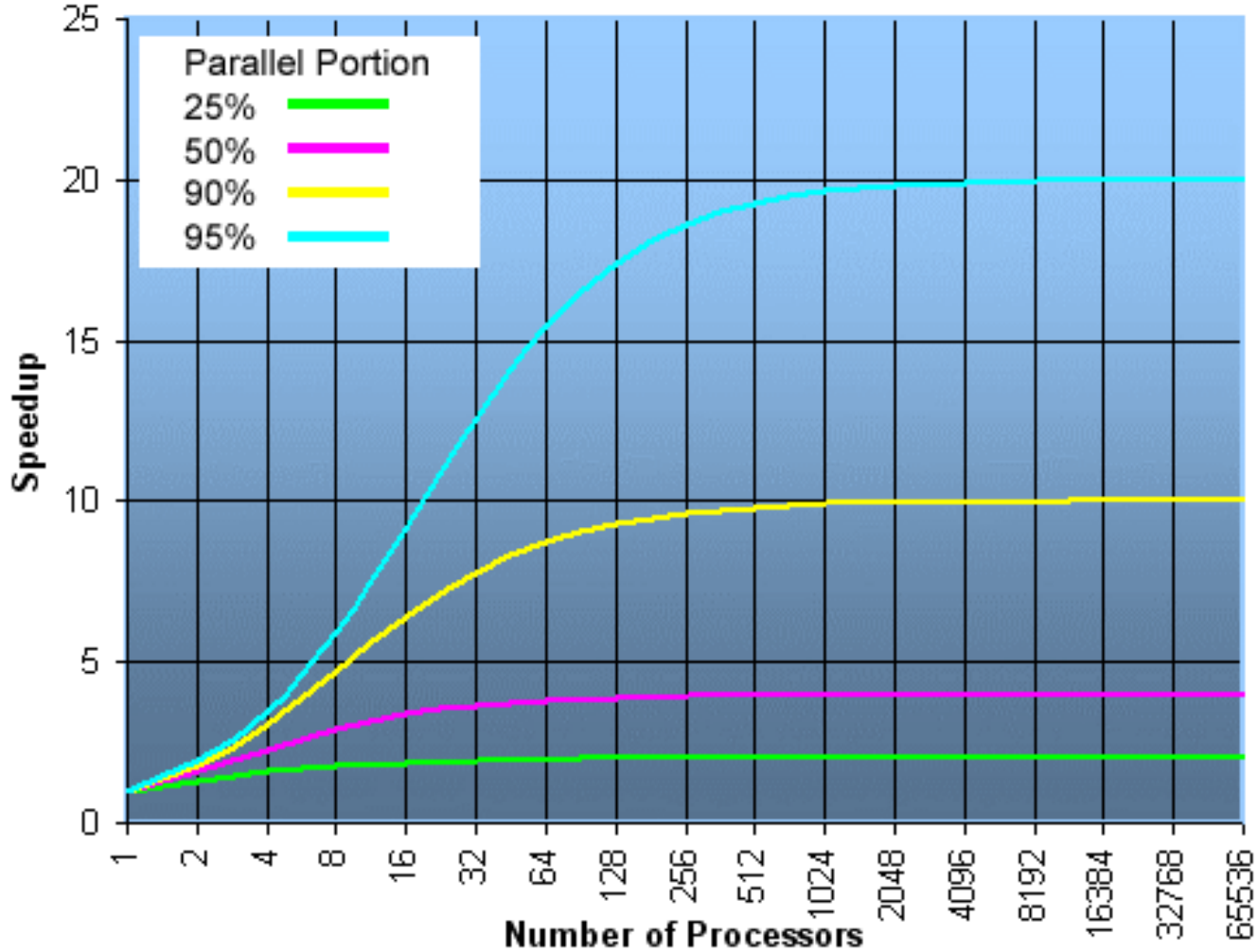
Matyash (treecode): CPP 08

Dejarnac: JNM, IEEE 09

- Includes ***nonlinear*** Coulomb collisions
- Includes neutral dynamics
- Includes impurity dynamics
- Massively parallel

Massively parallel simulations

Amdahl's Law for the maximum speed up due to parallelization (1967)



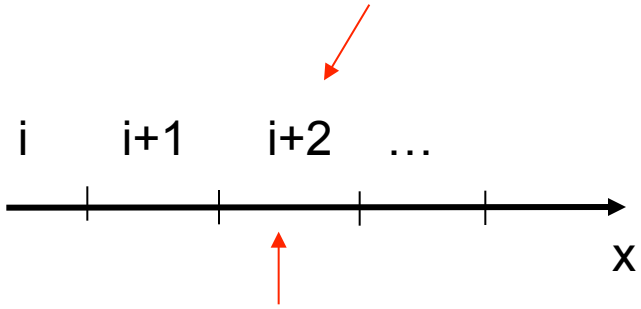
$$S = \frac{1}{1 - P}$$

S – speed up

P - parallel portion of the code

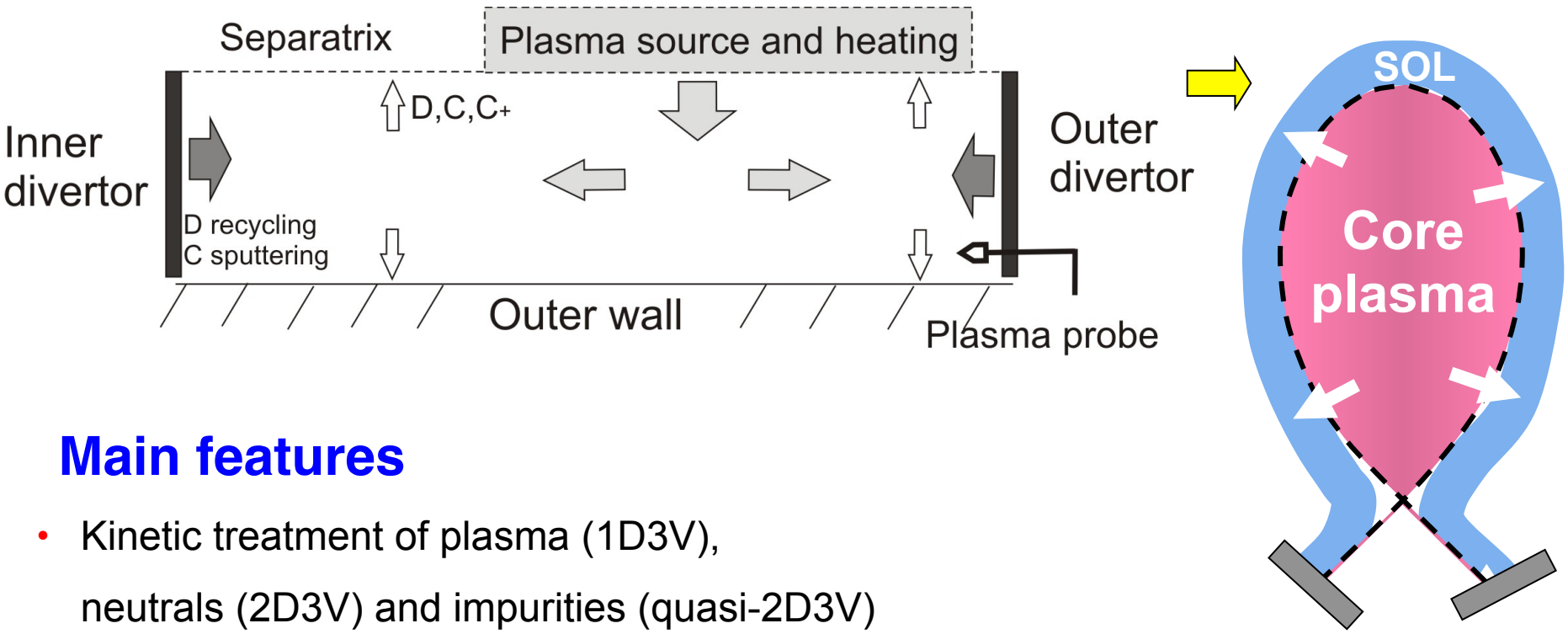
New structure of BIT1 code

„Natural sorting“: particles curry the cell index



- Neighboring particles in real space are neighbors in the computer memory: cache-hit increases [Tskhakaya JCP 2007]
- Cells are statistically independent: all collision probabilities are calculated separately, but are using the same random numbers
- Paralleling is straightforward
- Physics-based massively parallel Poisson solver [Tskhakaya IEEE 2010]

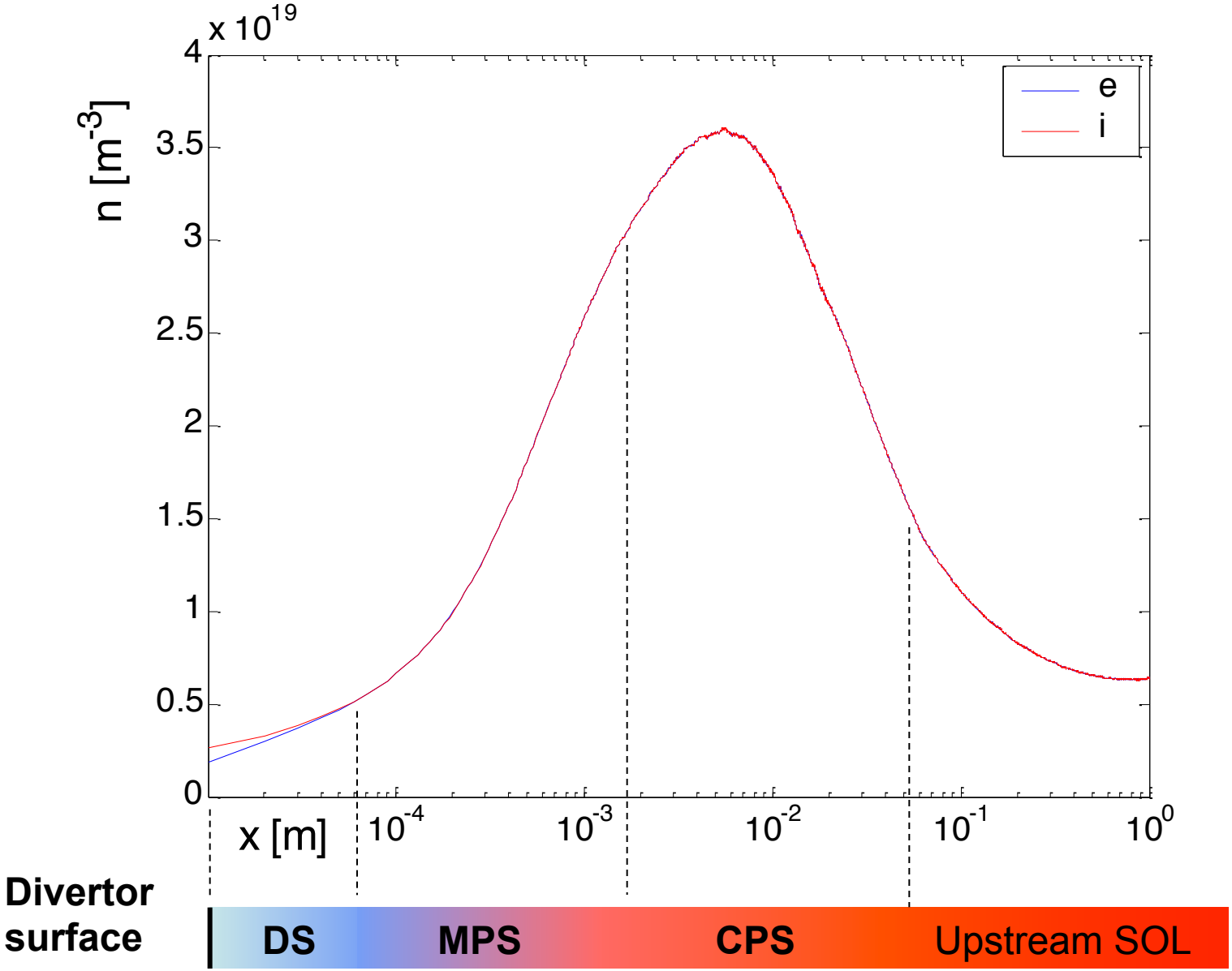
Electrostatic PIC/MC code BIT1



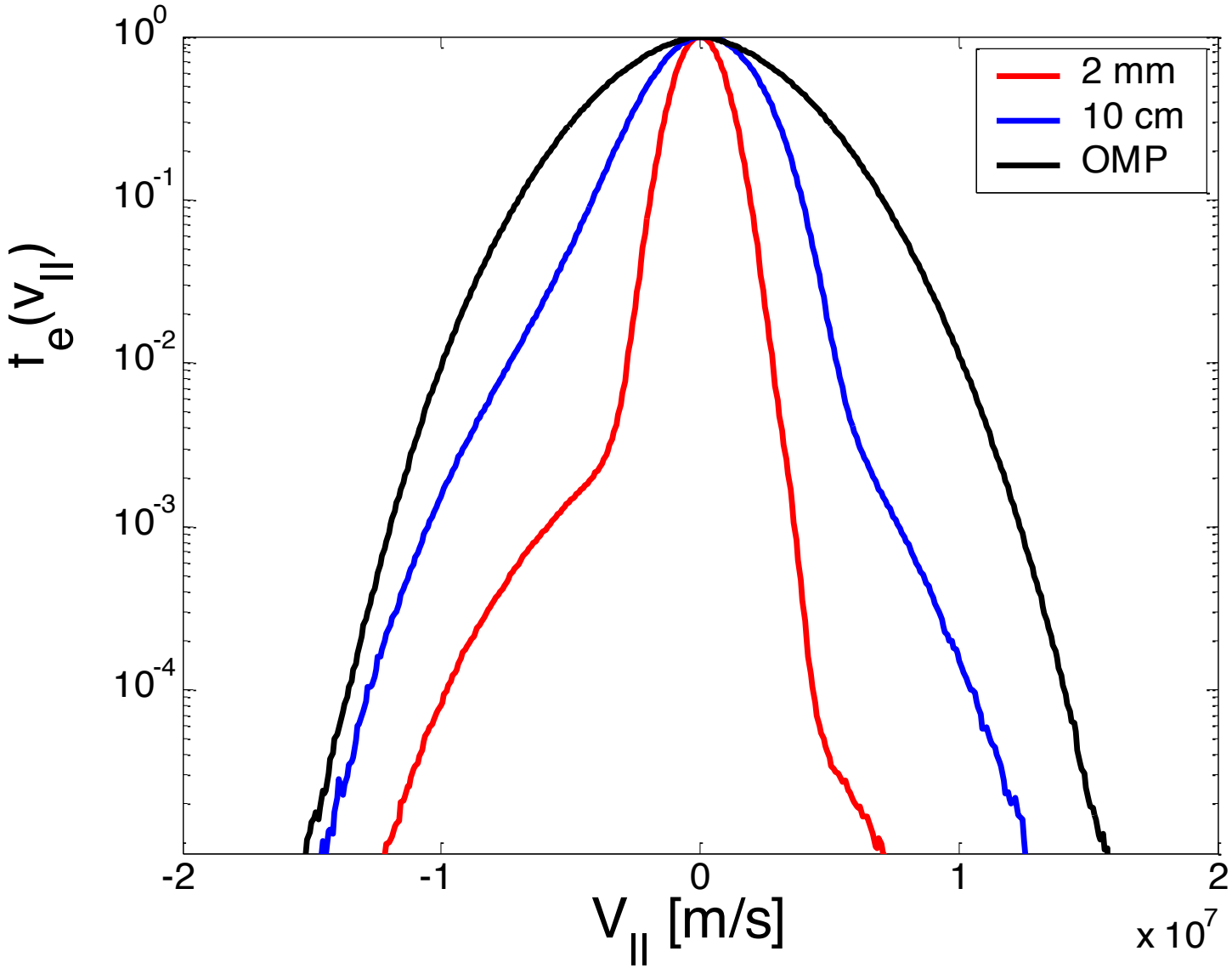
Main features

- Kinetic treatment of plasma (1D3V), neutrals (2D3V) and impurities (quasi-2D3V)
- Nonlinear energy and momentum conserving collision operators
- Linear model for plasma recycling and impurity (physical + chemical) sputtering.
- Massively parallel runs on 512 – 1024 processors
- $N_{particles}$ x N_{time} steps up to 10^{16}

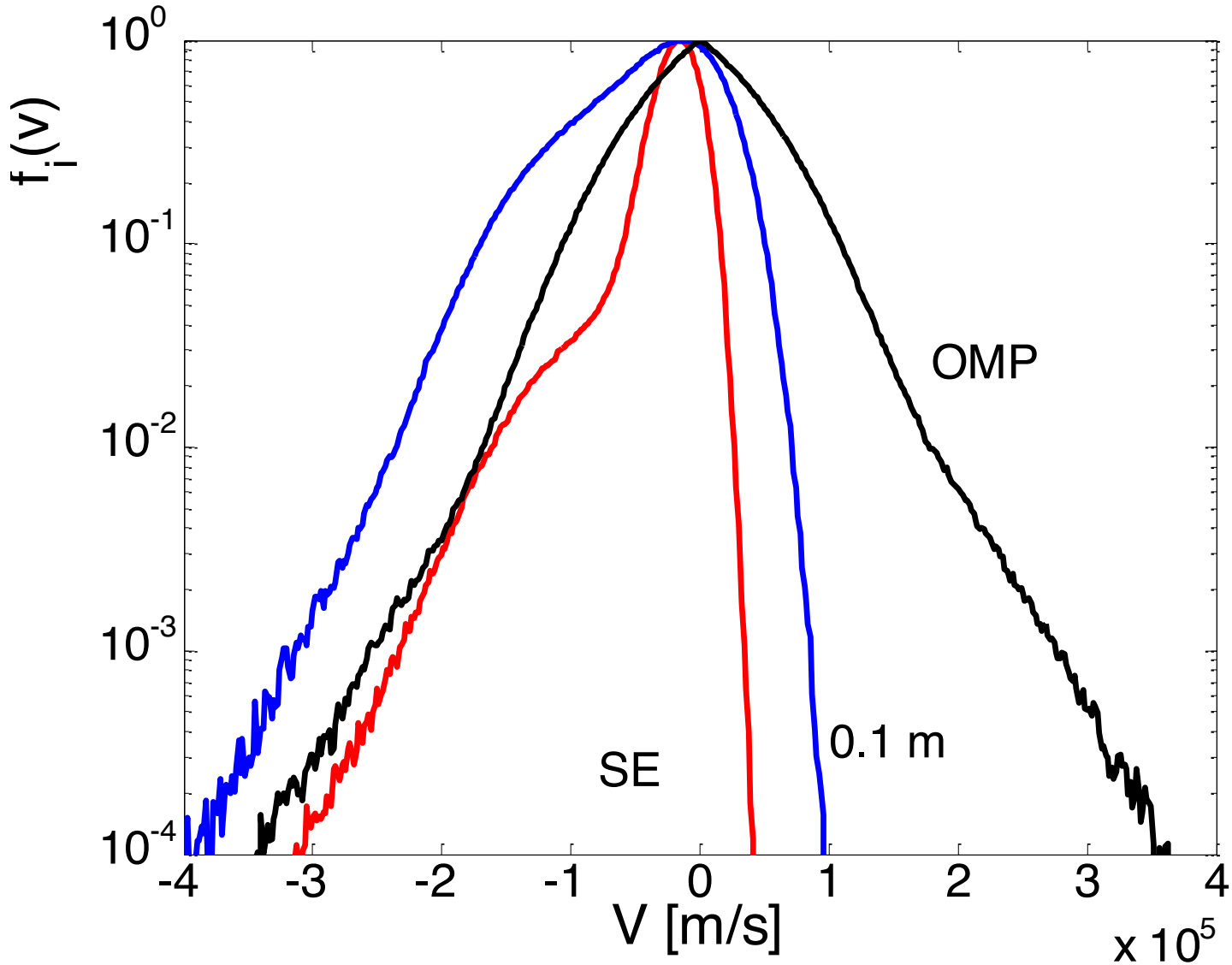
Plasma density profile at the AUG outer divertor



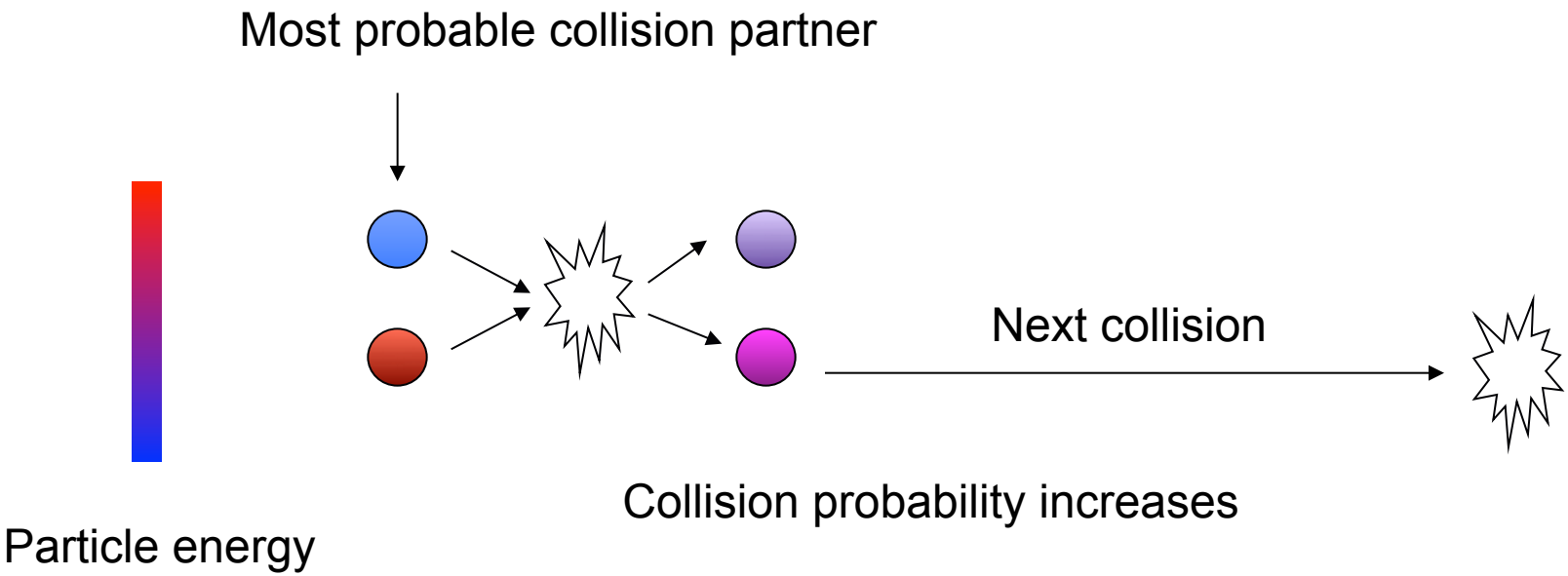
Parallel velocity distribution functions (el.)



Parallel velocity distribution functions (ion)

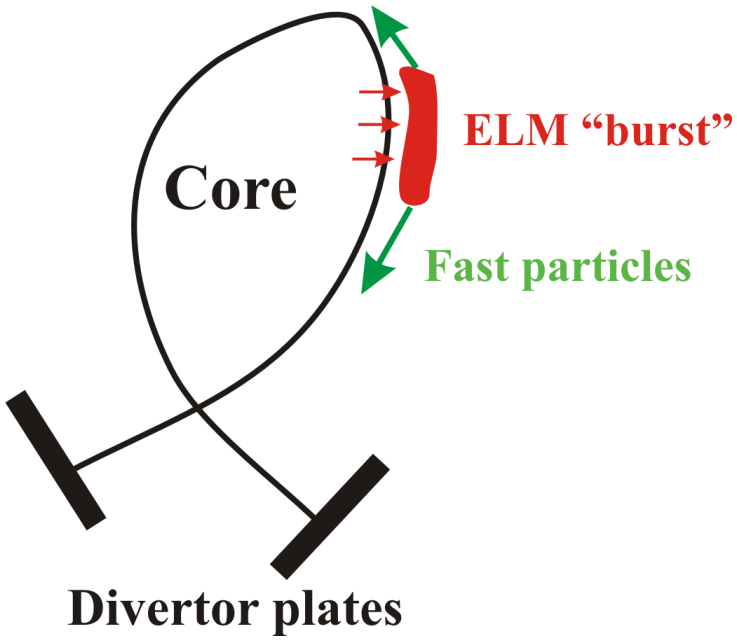


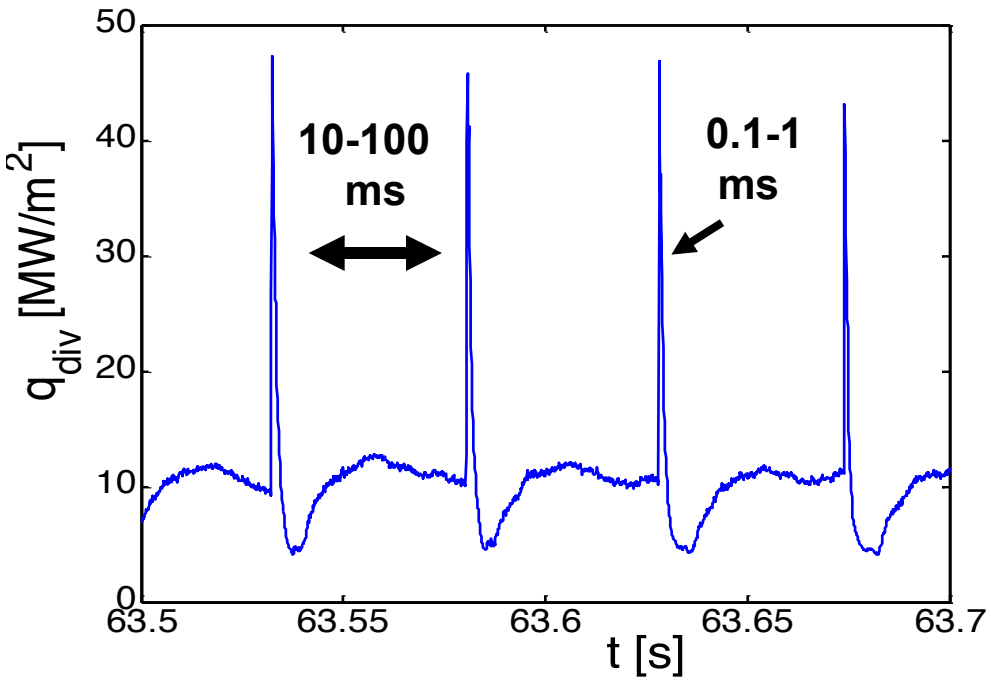
Parallel velocity distribution functions

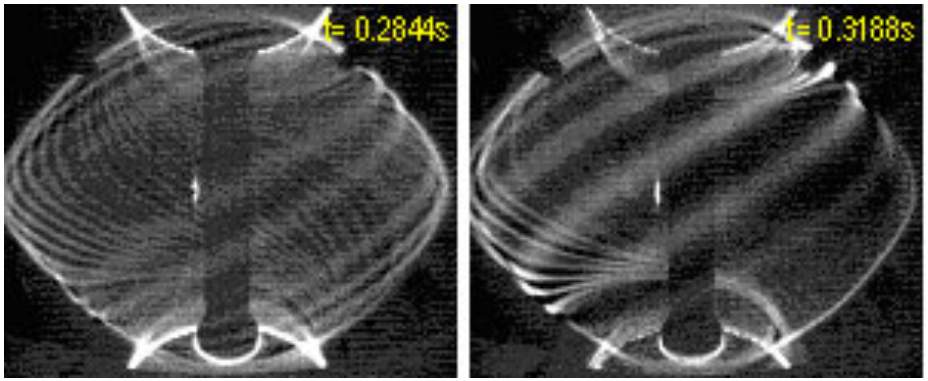


Particle either collide many times, or do not collide at all

Validation of the code: ELM simulations

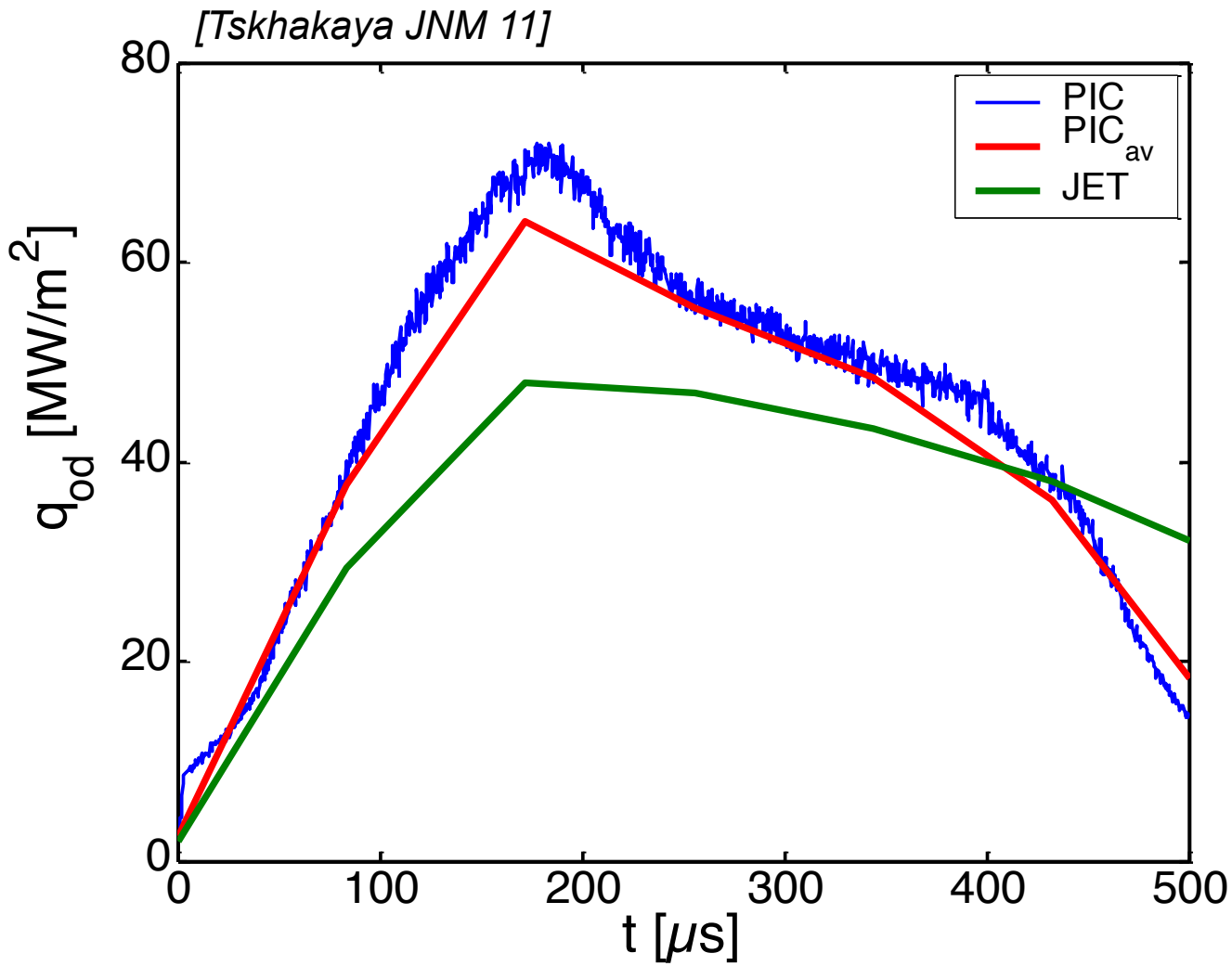






Filaments of small and large ELMs at MAST (UK)

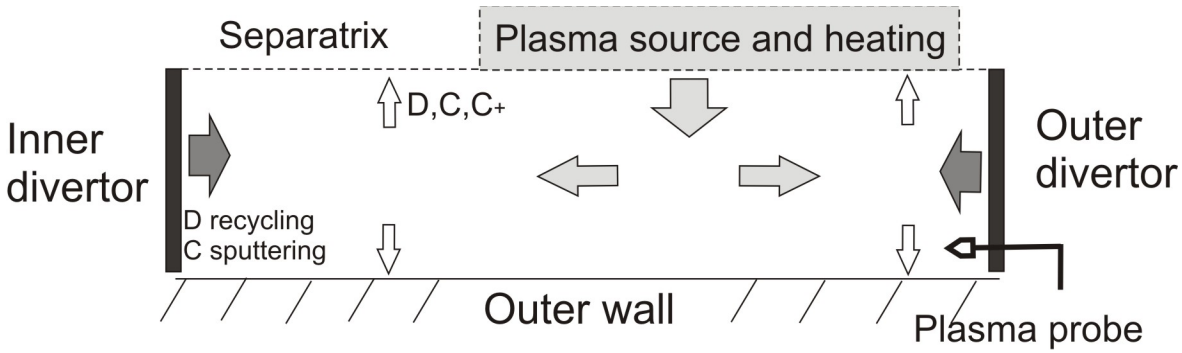
Comparison with experiment



Power loads to the OD plate during the 0.15 MJ ELM at JET (shot #74380).

Similar results for other shots at JET, TCV [Tskhakaya JNM09], AUG?

Simulation of high recycling SOL



Low recycling SOL: $S_{plasma} > 0,\ S_{heat} = 0,\ R_{recycling} << 1$

High recycling SOL: $S_{plasma} \sim 0,\ S_{heat} > 0,\ R_{recycling} \approx 1$

What is the fastest way to reach the stationary state?

Starting with high S_{plasma} later slowly reducing it

The final state depends on the way how it has been reached!

Modelling of the parallel transport

Parallel thermal force $F_{\|}^{T} = m_e \int V_{\|} C_{st} d\vec{V} \overset{?}{=} -0.71 n \partial_s T_e$

Ion sound speed $C_s = \sqrt{\dfrac{T_e + \chi T_i}{m_i}}, \quad \chi \overset{?}{=}$

Ion parallel viscosity $\pi_{\|}^{i} = m_i \int \left(U_{\|}^2 - U^2/3\right) f_i\left(\vec{V}\right) d\vec{V} \overset{?}{=} -\eta_{\|} \partial_s U_i$

Parallel heat flux $q_{\|} = \dfrac{m}{2} \int U_{\|} U^2 f\left(\vec{V}\right) d\vec{V} \overset{?}{=} -\chi_{\|} \partial_s T$

Power loads to the divertot plates

Plasma probe measurements

Simulation of Langmuir probes

There are a number indications that under some circumstances the T_e measured by Langmuir probes can significantly deviate from the actual values

Stationary SOL

Fussmann JNM 1984: $T_e^{LP} / T_e^{T.Scat} \approx 2$

Horacek JNM 2003: $T_e^{LP} / T_e^{B2} \approx 5$

Super-thermal electrons?

Assumption of bi-Maxwellian electron VDF:

Stangeby PPCF 1995, Van Rompuy PPCF 2007, Čerček JPFRS 2009…

ELMy SOL

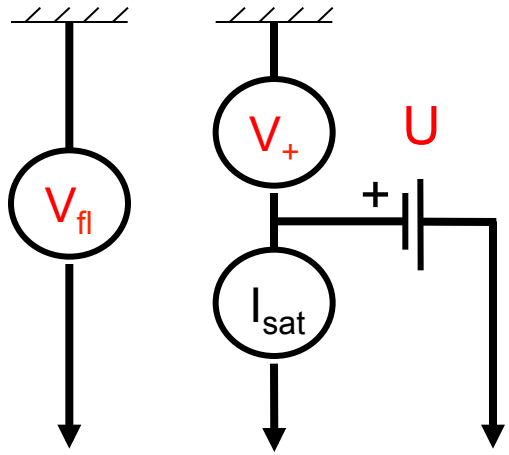
Herrmann JNM 2003, Kallenbach PPCF 2004, Pitts NF 2007, Tskhakaya JNM 2009 $\Big\}$ $T_e^{LP} / T_e^{sim} \sim 0.5$

ITER relevant

Modeling of the JET triple-probes [Tskhakaya JNM 2011]

Experiment

Triple probe



$$T_e^{TP} = \frac{V_{fl} - V_+}{\ln 2},$$

$$n = J_{sat}^i / eC_s, \quad q \approx 8 J_{sat}^i T_e,$$

$$C_s = \sqrt{2T_e^{TP} / M_i}, \; U >> T_e$$

Simulation

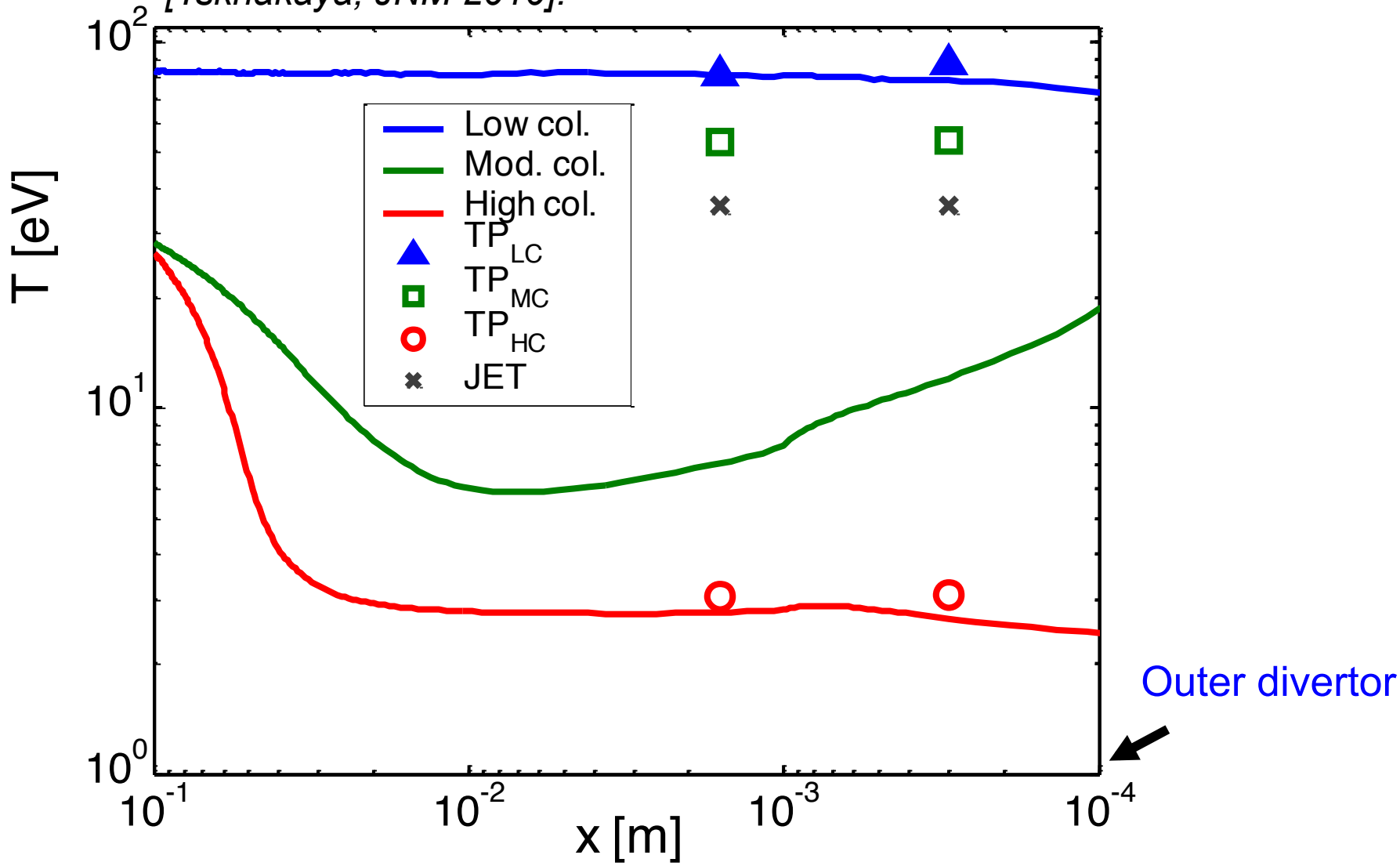
$$f_{e,i}(x, V_{\|}, t)$$

$$J_{sat}^i \equiv \int_0^\infty V_{\|} f_i(x, V_{\|}, t) dV_{\|} = \int_{\sqrt{2V_{fl}/m_e}}^\infty V_{\|} f_e(x, V_{\|}, t) dV_{\|},$$

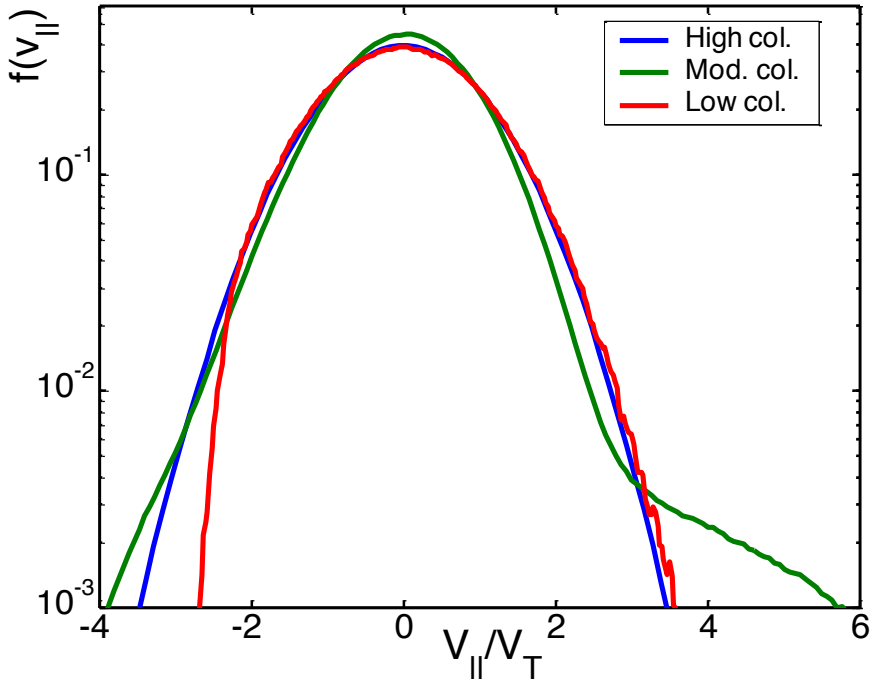
$$2J_{sat}^i = \int_{\sqrt{2V_+/m_e}}^\infty V_{\|} f_e(x, V_{\|}, t) dV_{\|} + \int_{\sqrt{2(V_+ + U)/m_e}}^\infty V_{\|} f_e(x, V_{\|}, t) dV_{\|}$$

Electron temperature profiles in the JET divertor plasma

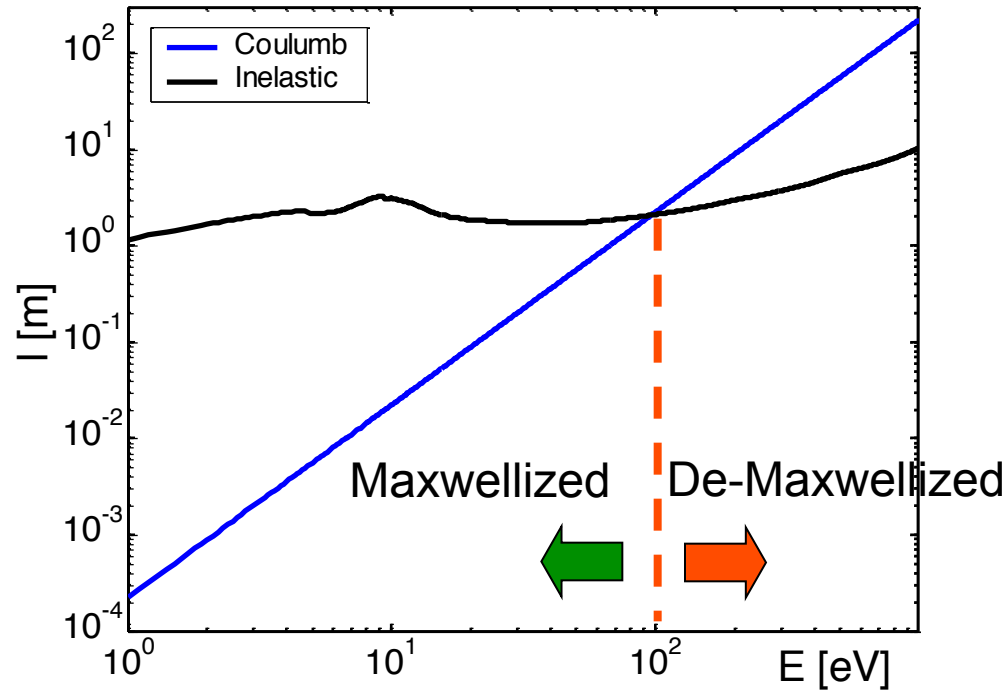
[Tskhakaya, JNM 2010].



Interpretation of probe measurements



Electron velocity distribution functions at the probe for different plasma recycling coefficients



Mean free paths for electron Coulomb and inelastic collisions near the divertor

Ion sound speed

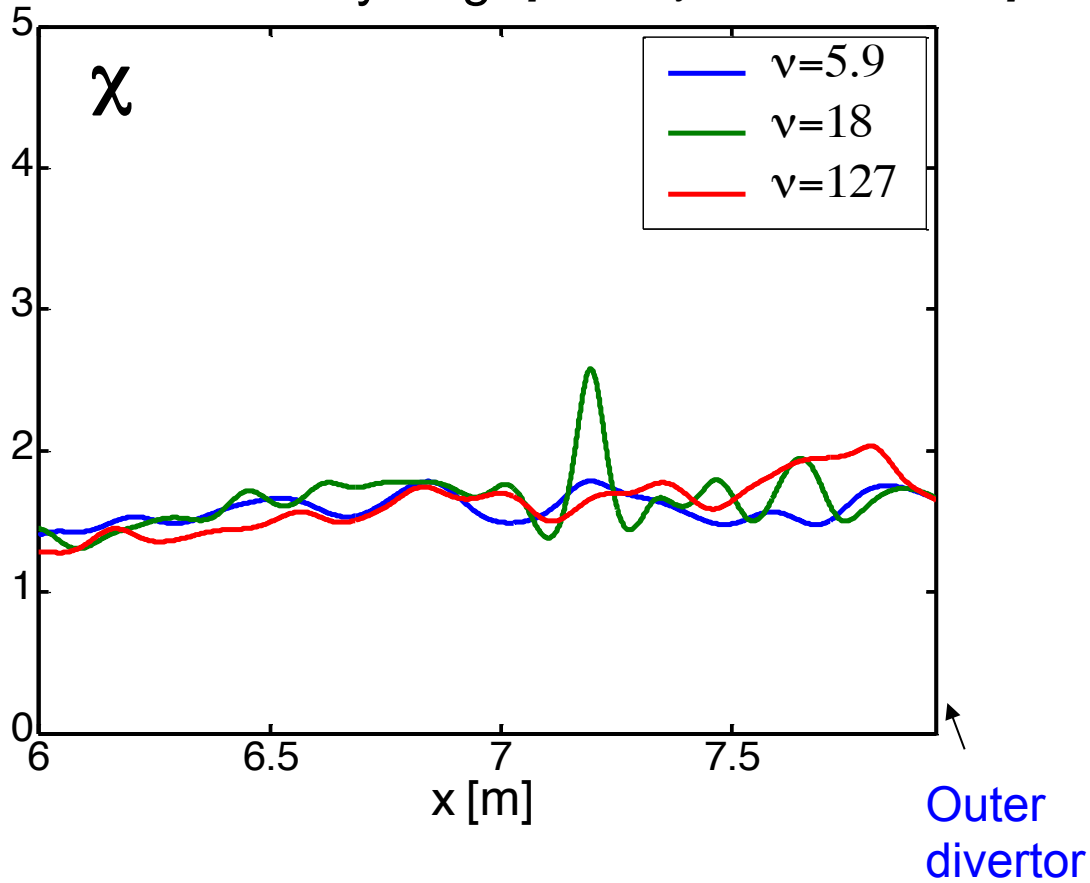
$$C_s = \sqrt{\frac{T_e + \chi T_i}{m_i}}$$

$$T_i \sim n_i^{\chi-1}$$

Usual assumption

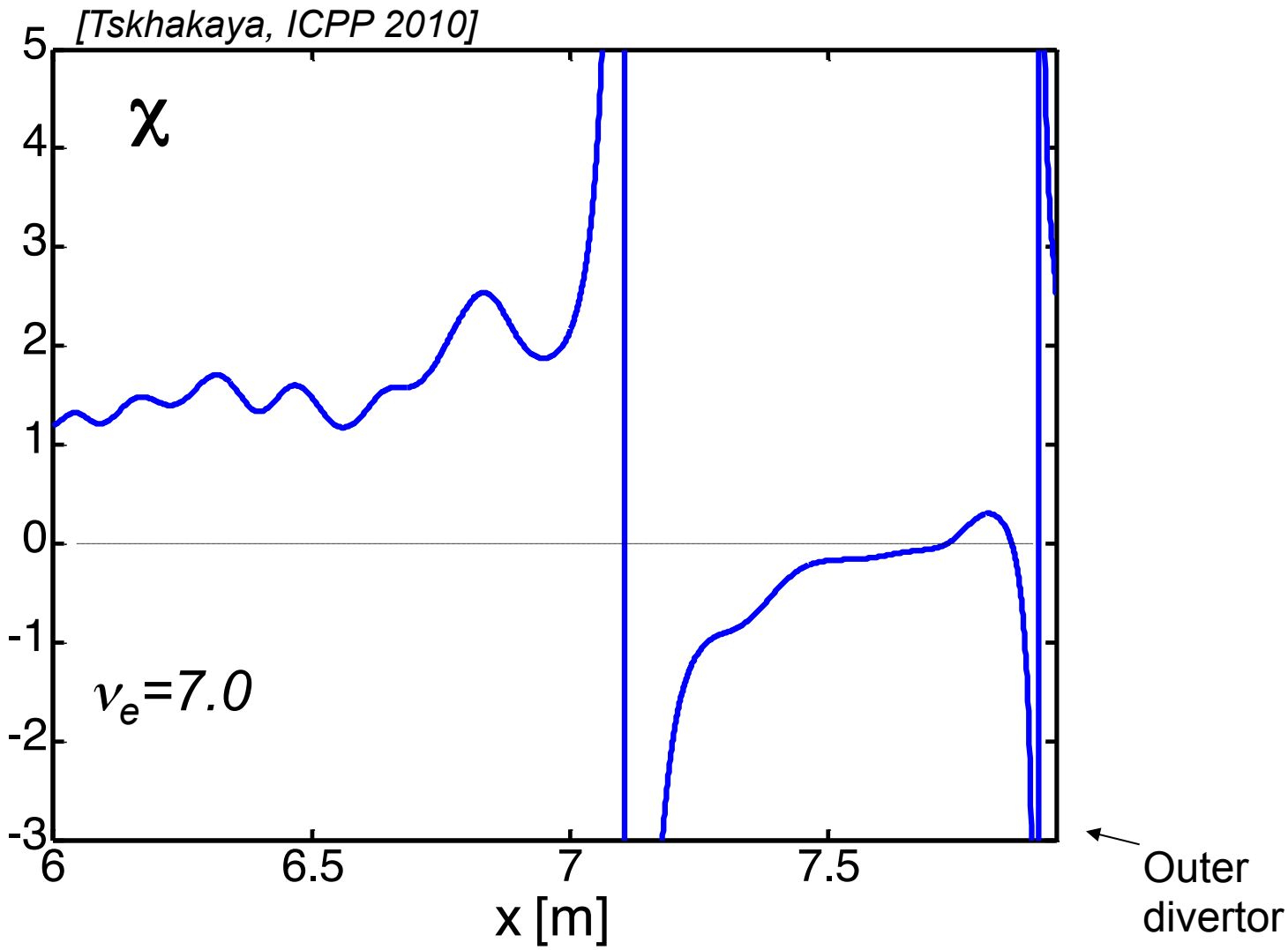
$$1 \le \chi \le 3$$

Case w/o recycling *[Tskhakaya EU-PWI TF 2010]*



Poloidal profiles of the polytropic coefficient for different SOL collisionalities.

Ion sound speed (high recycling SOL)



Poloidal profile of the polytropic coefficient.

Ion sound speed (high recycling SOL)

$$T \sim n^{\gamma-1}$$

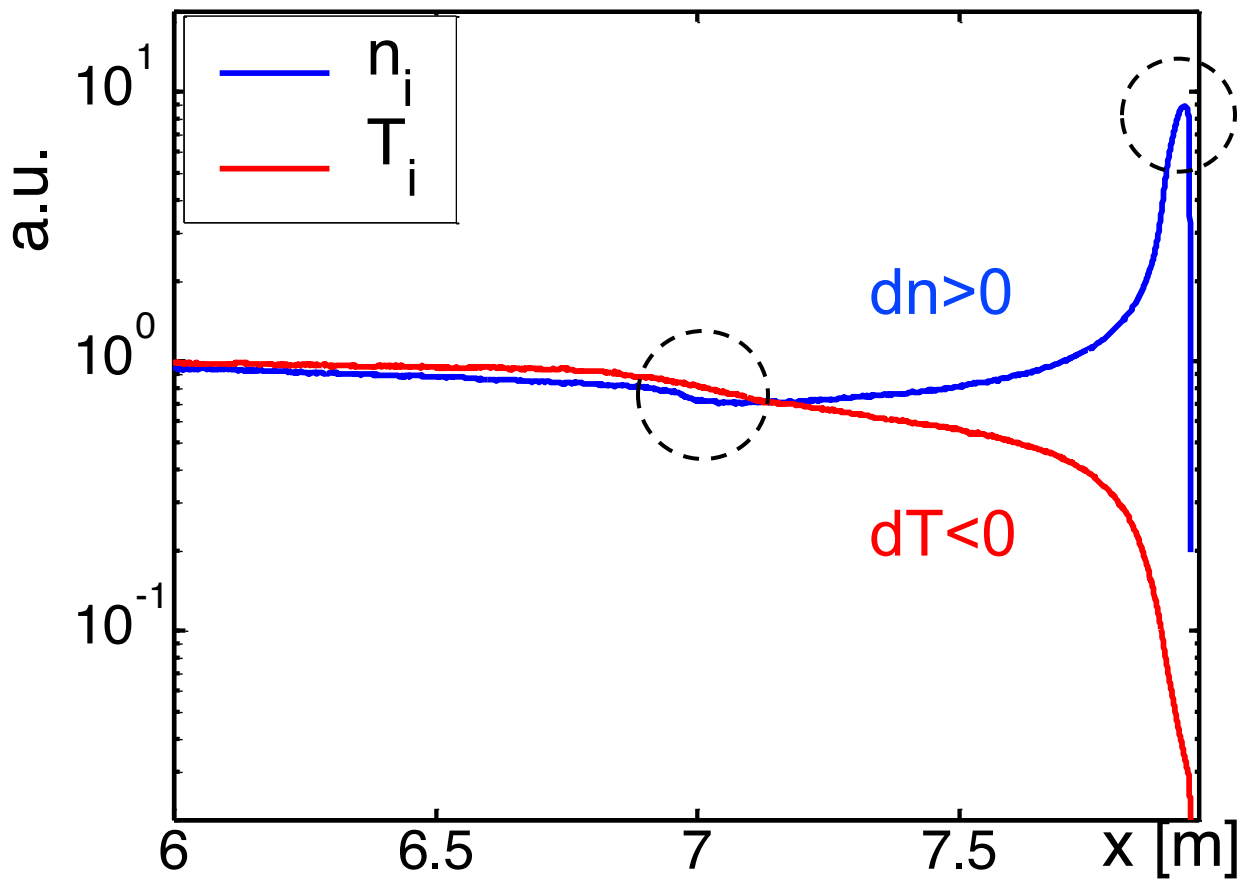
$$\Downarrow$$

$$\chi = 1 + \frac{d \ln T}{d \ln n}$$

How can we define the ion sound speed?

$$C_s = \sqrt{\frac{T_e + \langle \chi \rangle T_i}{m_i}}$$

[Tskhakaya, ICPP 2010]



Poloidal profiles of the ion density and temperature.

Parallel heat flux (low recycling SOL)

Limited expression of the heat flux

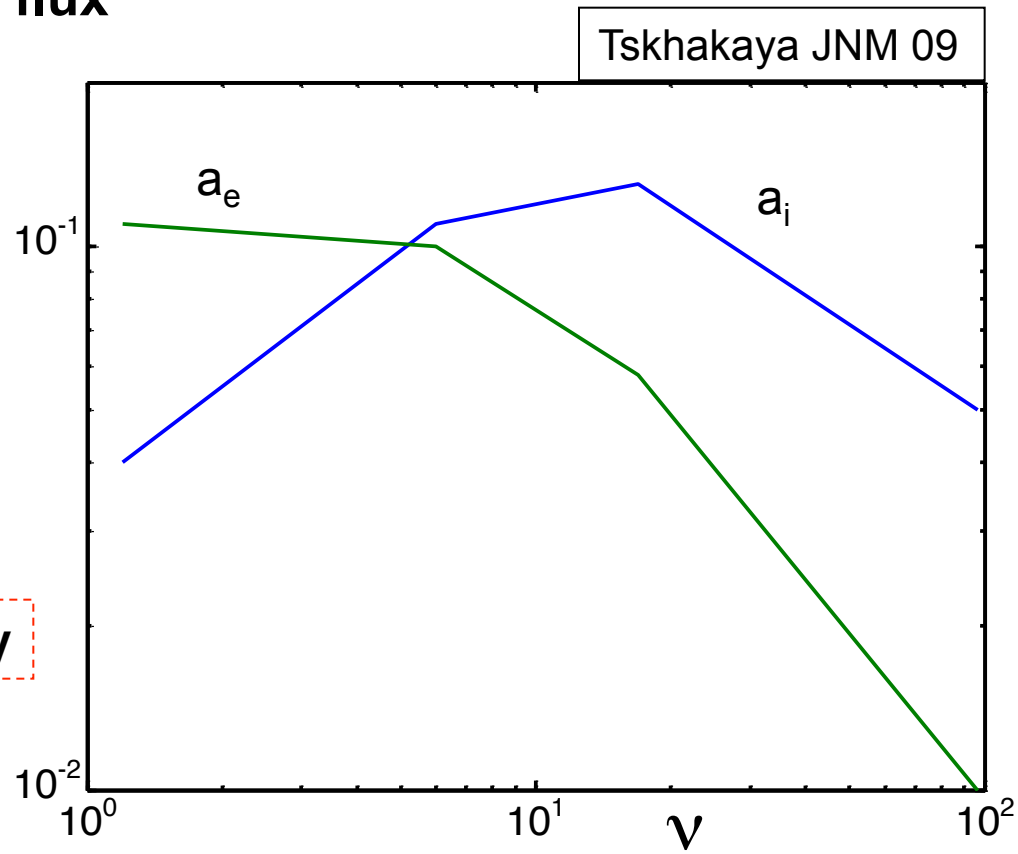
$$q_{\parallel} = \left(\frac{1}{q_{SH}} + \frac{1}{\alpha q_{FS}} \right)^{-1}$$

α is a free parameter (0.03 – 1.0)

Depends strongly on collisionality

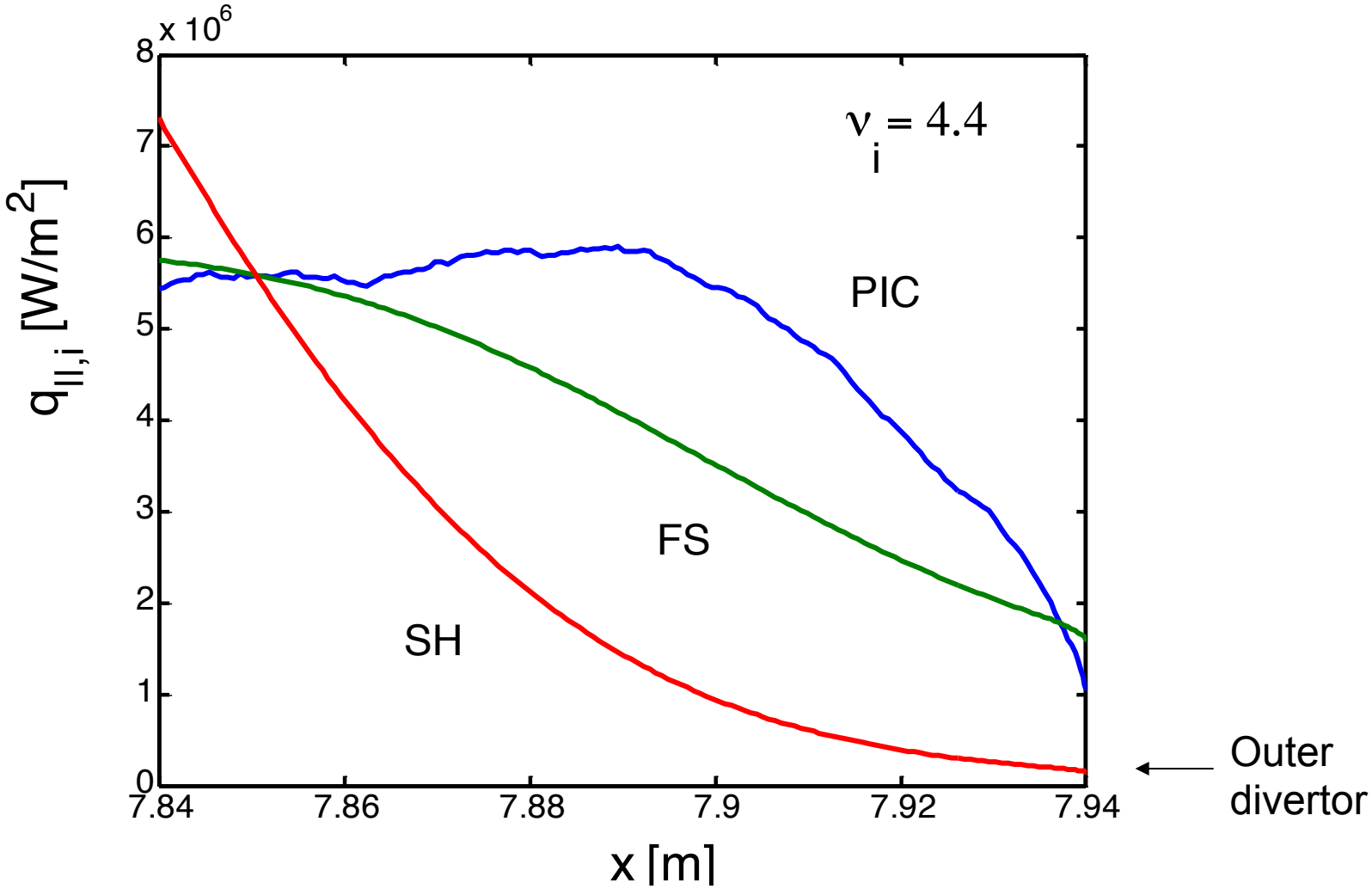
$$q_{SH} = -\kappa_{\parallel} \frac{\partial T}{\partial s}$$

$$q_{FS} = n V_T T$$



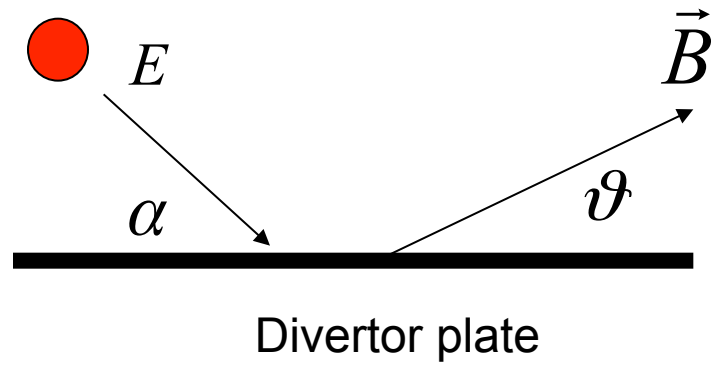
Heat flux limiting factors vs. plasma collisionality

Parallel heat flux in the attached high recycling divertor plasma



Poloidal profile of the ion heat flux for JET relevand parameters. FS and SH denote the Spitzer-Härm and the free streaming heat fluxes.

Average energy and incident angle of ions impinging to the DP



Analytical/numerical models

$$\langle E \rangle = 2T_i + e\varphi_{sheath}$$

$\alpha = \vartheta - 10°$ Collisionless PIC [Chodura 1986]

$40° \le \alpha < 65°$ for $\vartheta \sim 5° \div 10°$

FP with BGK operator [Devaux PPCF 2008]

Simulation results for JET-relevant SOL

ν_i	Divertor		$\langle E \rangle$	$\langle E \rangle$	α
4.4	Inner	D+	22.4	19.0	50.1
		C+	40.8	18.2	60.8
	Outer	D+	18.0	13.1	49.9
		C+	36.3	12.3	60.9
2.3	Inner	D+	91.2	72.2	43.0
		C+	90.6	70.0	37.0
	Outer	D+	55.1	39.8	46.2
		C+	61.1	37.8	45.3

For high collisionality there is strong main ion-to-impurity coupling leading increased impurity fluxes

The main problem for our simulations:

Results are sensitive to the A&M and PSI data, and most (!) of this data is missing.

A&M

$e + W^{(i)} \rightarrow e + W^{(i)*}$

$e + W^{(i)} \rightarrow 2e + W^{(i+1)}$

$2e + W^{(i)} \rightarrow e + W^{(i-1)}$

$H + W^{(i)} \rightarrow H^{+} + W^{(i-1)}$

$H^{+} + W \rightarrow H + W^{+}$

PSI

H on W, W sputtering

W self-sputtering

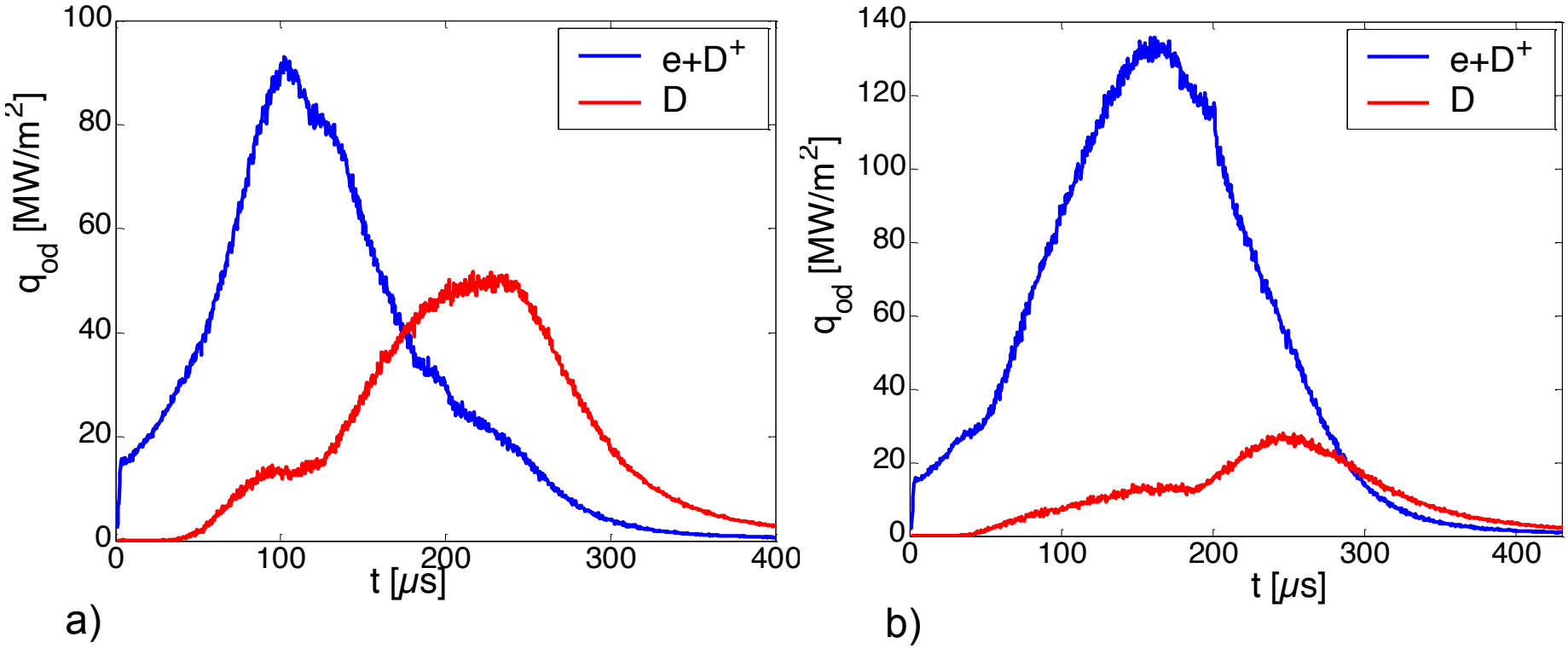
H on W, release of H

W on W, reflection

H= H, D, T

- Implemented in BIT1
- data expected
- no data is expected

Sensitivity of simulation results to the implemented PSI data



Power loads to the outer divertor during 0.15 MJ type-I ELM at JET #74380.

a) Constant recycling coefficient R_D= 0.99;

b) Energy-dependant $R_D(E)$.

Formulation of the boundary condition for ion velocity at the SE

Conventional model

$$\frac{\partial}{\partial s} nV = S_p$$

$$\frac{\partial}{\partial s} n\left(m_i V^2 + T_e + T_i\right) = -m_i V S_m$$

$$T_i \sim n^{\gamma - 1}$$

$$\Downarrow$$

$$\left(c_s^2 - V^2\right)\frac{\partial}{\partial s} V = V^2 \frac{S_m + S_p}{n} + c_s^2 \frac{S_p}{n} > 0$$

$$c_s = \sqrt{\frac{T_e + \chi T_i}{m_i}}$$

$$\Downarrow$$

At the SE $\boxed{V = c_s, \quad \frac{\partial}{\partial s} V \to \infty}$

But

- c_s is not well-defined
- for $\gamma \neq 1$

$$\frac{\partial}{\partial s} T_i \to \infty$$

Is this physical?

Drop/increase of physical quantities across the plasma sheath

$$\frac{n_w}{n_{SE}} = \left(\frac{V_w}{V_{SE}}\right)^{-1} \approx \exp(-\psi_0),\ \psi_0 \approx \ln\sqrt{\frac{m_i}{2\pi m_e}} \sim 2 \div 5,$$

For perfectly magnetised electrons and ions (!) we obtain

$$T_{e,w} = T_{e,SE}\left(1 - \frac{2}{3\pi}\right), \qquad T_{i,w} = T_{i,SE}\frac{1}{3}\left(2 + \left(\sqrt{1+2\psi_0} - \sqrt{2\psi_0}\right)^2\right)$$

For $\psi_0 \approx 3$

$$\frac{n_w}{n_{SE}} = \left(\frac{V_w}{V_{SE}}\right)^{-1} \sim 0.05,\ \frac{T_{e,w}}{T_{e,SE}} \sim 0.85,\ \frac{T_{i,w}}{T_{i,SE}} \sim 0.68$$

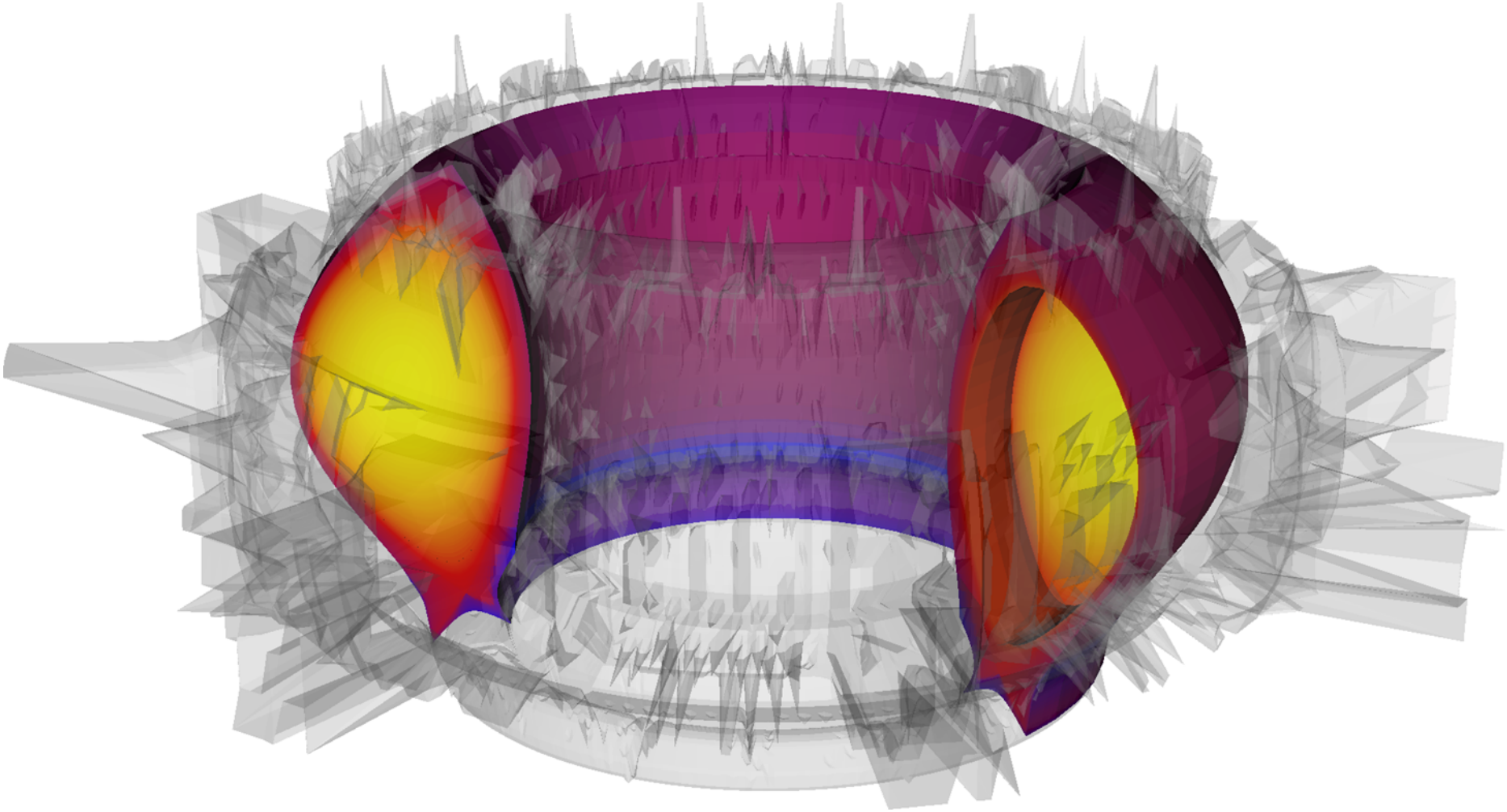
$$V_{SE} = \sqrt{\frac{T_e + T_i}{m_i}}$$

$$\frac{d\ln T}{d\ln n} << 1 \quad \Rightarrow \quad \chi_{SE} = 1 + \cancel{\frac{d\ln T}{d\ln n}} = 1$$

Conclusions

- Massively parallel PIC modeling is a powerful tool for SOL study
- Parallel transport coefficients in the high recycling SOL strongly deviate from the classical ones.
- Sound speed is NOT a well-defined value
- The ion parallel heat flux can exceeds the Spitzer-Harm and free streaming heat fluxes
- Development of new analytic/empirical models is required. E.g. boundary condition for the ion parallel speed has been revised.
- Classical expressions systematically underestimate average energy of ions impinging to the DP in the high recycling attached divertor plasma
- Future work: development of higher dimensional massively parallel codes
- We have (very) long way to go

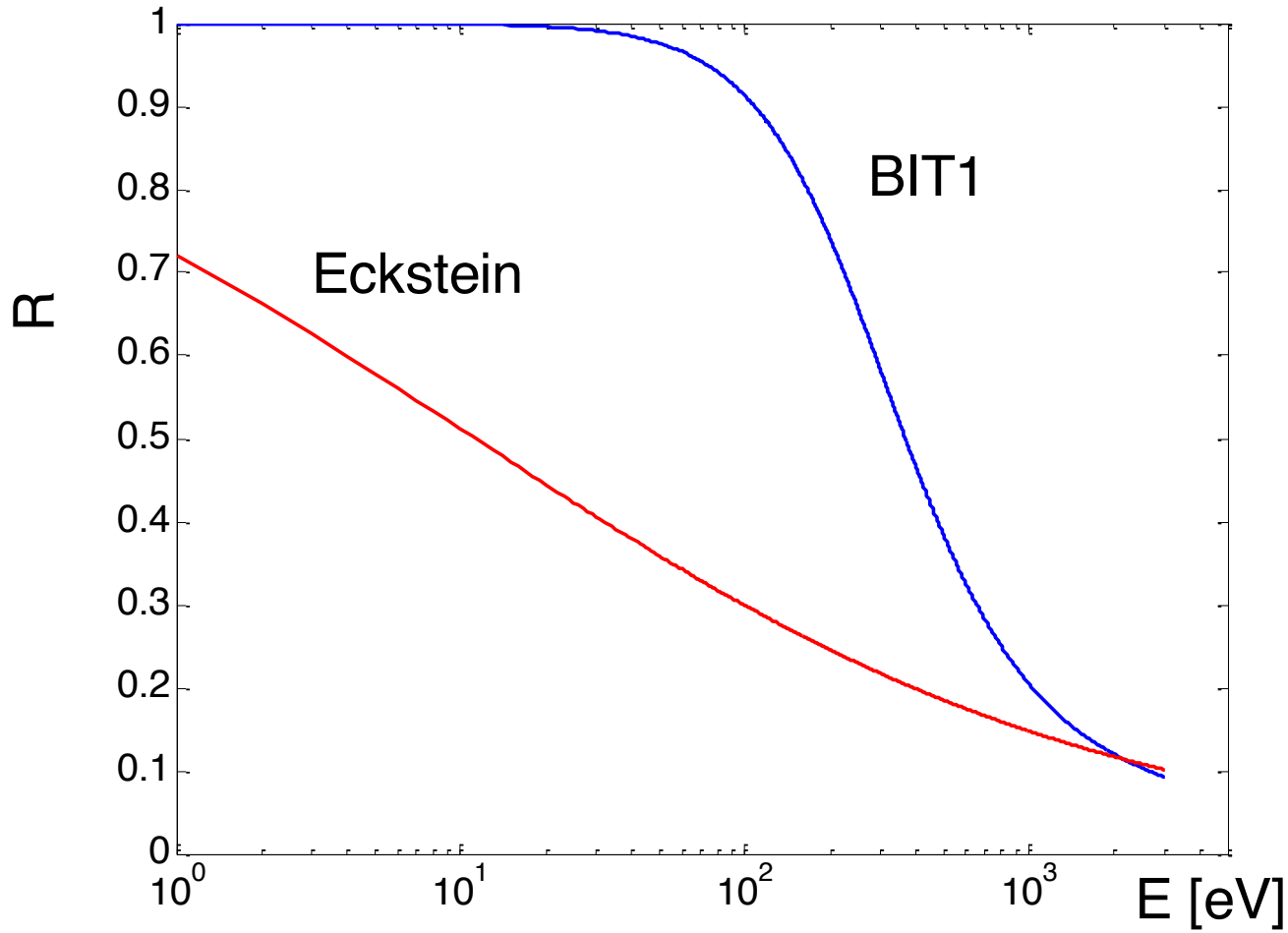
EU Integrated Tokamak Modeling TF



Test simulation of AUG. Figure is kindly provided by

H.J. Klingshirn, D. Coster, T. Lunt and T. Koskela

Sensitivity to A&M and PSI data



D reflection coefficient for D+/D impact on C.

"Eckstein" corresponds to the model from [Eckstein, NF 84].

$$f_e\left(\vec{V}\right) = \frac{n_0}{V_{T,e}^3 (2\pi)^{\frac{3}{2}}} \frac{2}{1 + erf\left(\sqrt{\psi_0}\right)} \exp\left(-\frac{V^2}{2V_{T,e}^2} + \psi - \psi_0 \right) H\left(V_{\parallel} - V_c\right),$$

$$V_{T,e} \equiv \sqrt{\frac{T_e}{m_e}}, \; V_c \equiv \sqrt{\frac{2e\varphi}{m_e}}.$$

$$V_{T_i,w} \sim V_{T_i} \left(\sqrt{1 + 2\psi \frac{T_e}{T_i}} - \sqrt{2\psi \frac{T_e}{T_i}} \right) \approx V_{T_i} \left(\sqrt{1 + 2\psi} - \sqrt{2\psi} \right)$$

Differential cross-sections

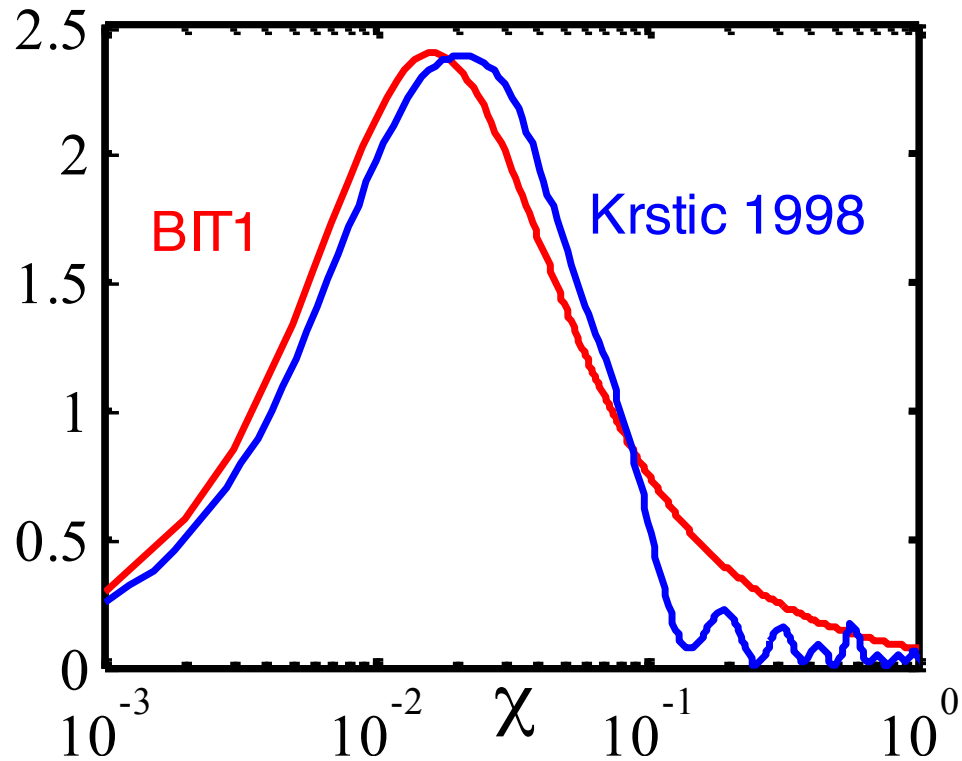
$$\frac{d^3\sigma_{ion}}{dE_s d\Omega_s d\Omega_p} = \frac{d\sigma_{ion}}{dE_s}\left(E_p, E_s\right)\frac{d\sigma_{ion}}{d\Omega_s}\left(E_s, \cos\Theta_s\right)\frac{d\sigma_{ion}}{d\Omega_p}\left(E_p, \cos\Theta_p\right)$$

$$\frac{d\sigma_{ion}}{dE_s}\left(E_p, E_s\right) = \frac{a}{E_p + E_0}\left[\frac{1}{\left(1+\varepsilon_s\right)^2} + \frac{1}{\left(\varepsilon_p - \varepsilon_s\right)^2} - \frac{1}{\left(1+\varepsilon_s\right)\left(\varepsilon_p - \varepsilon_s\right)} + \ln\varepsilon_p \sum_{i=0}^{3}\frac{b_i}{\left(1+\varepsilon_s\right)^{3+i}}\right],$$

$$\frac{d\sigma_{ion}}{d\Omega} = \frac{1}{4\pi\ln\left(1+\alpha E\right)}\frac{\alpha E}{1+\alpha E\sin^2\left(\chi/2\right)},$$

$$\varepsilon_p = E_p / E_0, \quad \varepsilon_s = E_s / E_0,$$

$e + H = 2e + H^+$



Angular differential cross sections