INSTITUTE OF PLASMA PHYSICS
OF THE CZECH ACADEMY OF SCIENCES

Introduction to different numerical methods used in Magnetic Confinement Fusion Plasmas

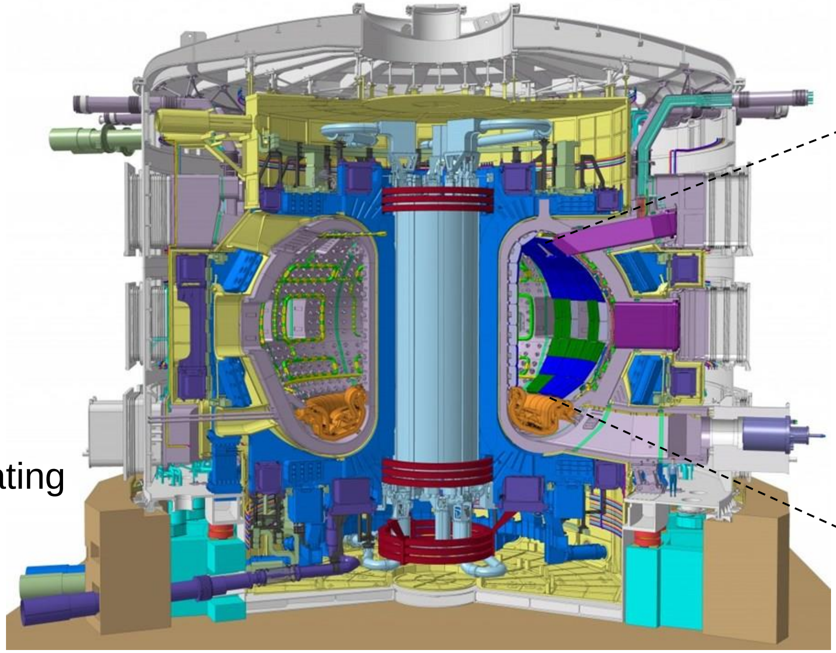
D. Tskhakaya

Institute of Plasma Physics of the Czech Academy of Sciences, Prague, Czech Republic

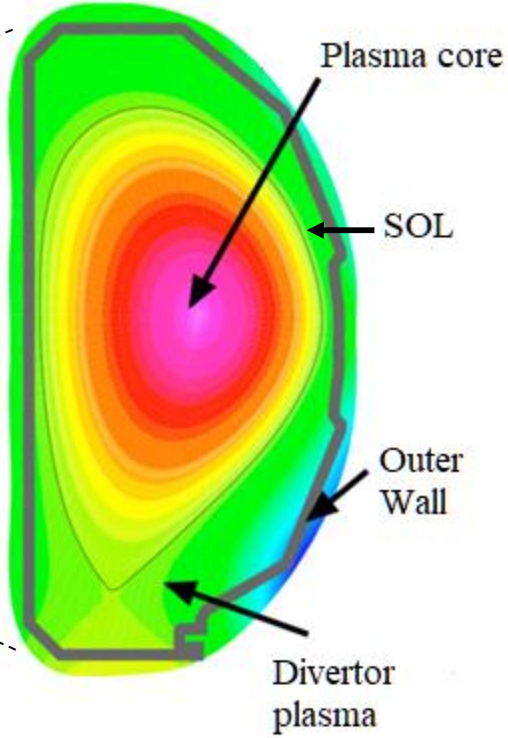
MINISTRY OF EDUCATION,
YOUTH AND SPORTS

Different methods for MC fusion plasma study

RF heating



NBI heating



Plasma-surface interaction (< 1eV, nm, 10^{-14} s – 1 year)

- Monte Carlo (MC)
- Molecular dynamics
- Other methods for studying arcing, surface morphology, neutron irradiation damage, …

SOL (1-100 eV, 1-100 mm, 10^{-5} – 10^{-2} s)

- (gyro-)Fluid
- Gyrokinetic
- Full kinetic
- Monte Carlo

Plasma core (> 1 keV, 1-100 cm, 10^{-3} – 1 s)

- MHD (transport/equilibrium)
- Gyrokinetic (GK)
- Runaway Electron transport

Plasma heating (~MeV, 1 – 100 cm, 10^{-4} – 1 s)

- NBI codes (MC)
- RF heating and current drive (MC, Maxw. S, RayT., GK)

Outline

- Introduction
- Different models
  - Monte Carlo models for neutral particles

  Questions
  - Impurity transport codes
  - Particle-in Cell (PIC codes)

  Questions
  - Drift- and Gyro-kinetic

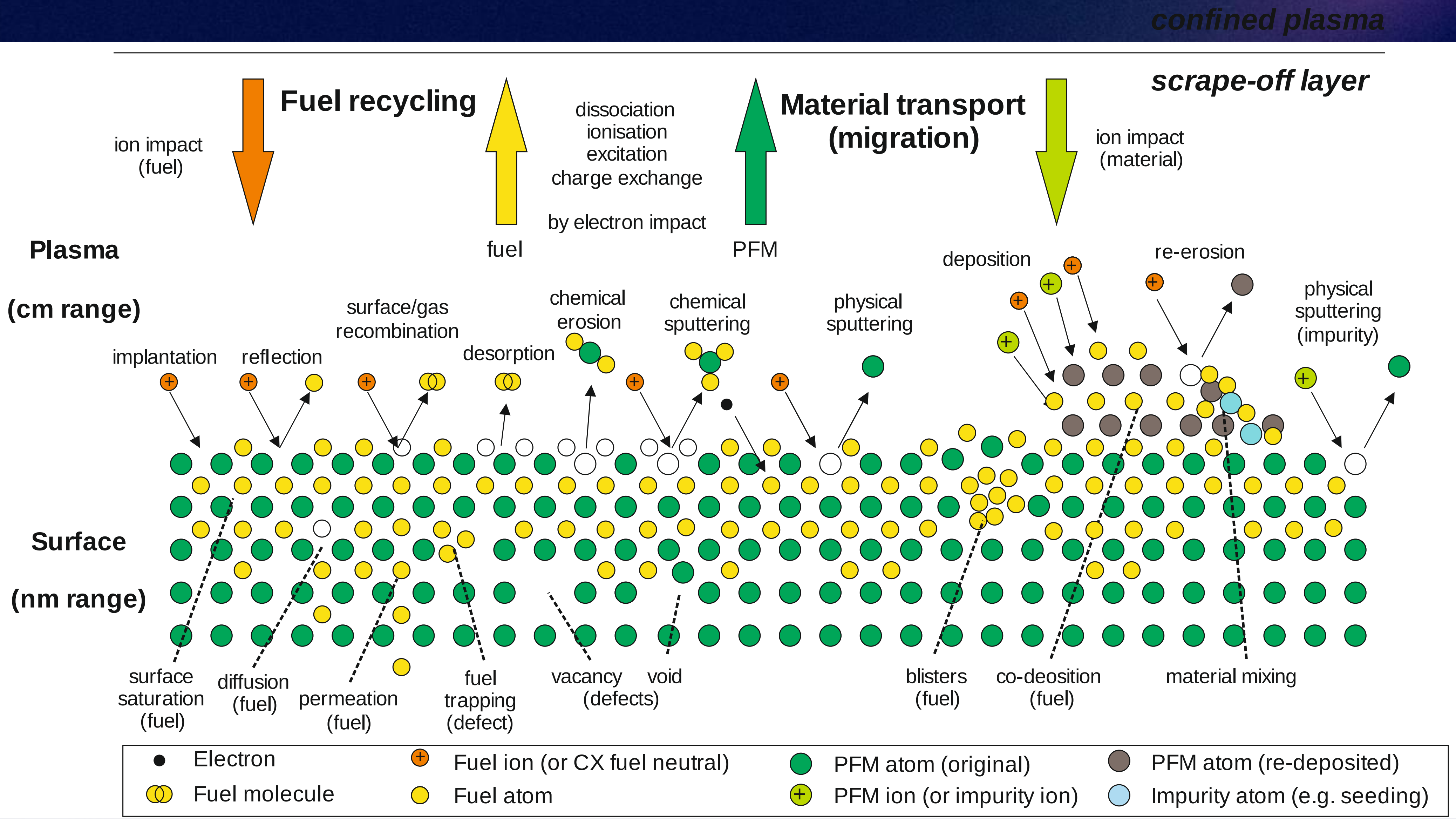
  Questions
  - Fluid (static and turbulence)

  Questions
  - Plasma Magnetohydrodynamics (MHD)

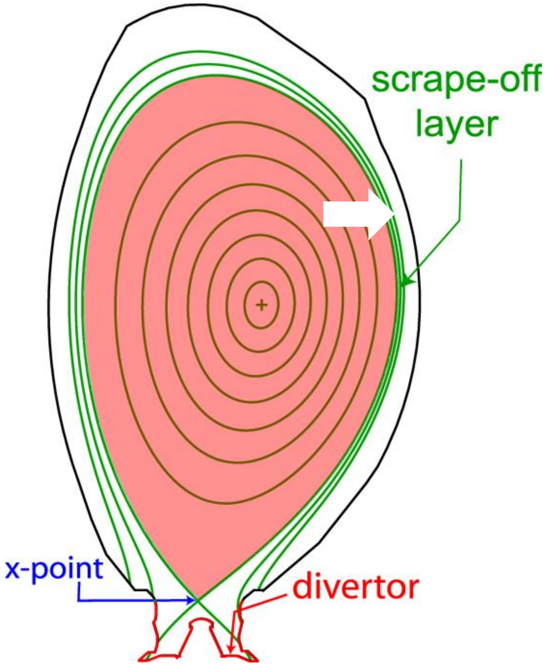
  Questions
- On next lectures

Plasma wall interactions in MCFP

S. Brezinsek,
30th EFPW, 2023

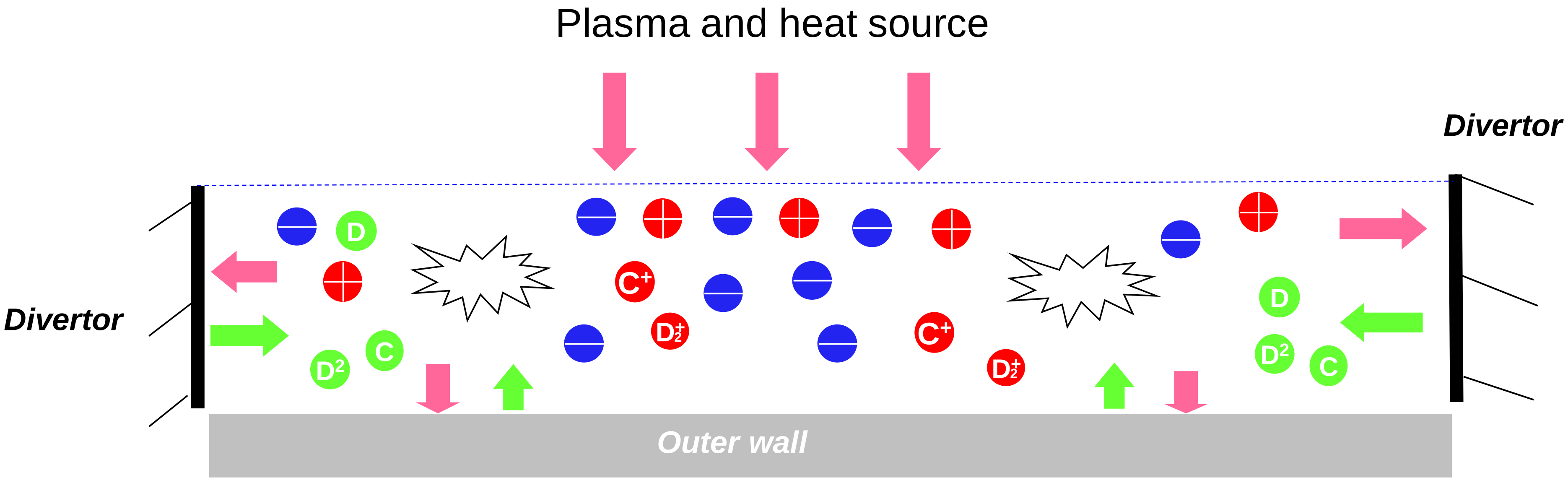


SOL modelling



For each problem one has to answer the following quetions

- Which model is is applicable
- What are the limitations of this model



SOL content and related physical processes

SOL content

- Main ions (typically): H^+, D^+, T^+
- Neutral particles recycled from PFC: H, D, T
- Low energy fusion products: He^{+i}
- Intristic impurity: W, C, F, O_2, ... (PFC material, „parasitic“ leaks, ets)
- Seeded impurity: Ne, Ar, N, ...
- Dust particles: 1 ~ 100 µ

Main processes

- Parallel transport
- Classical cross-field transport: diffusion, drifts
- Anomalous transport: turbulent, intermittent transport (blobs, ELMs)
- Atomic and molecular processes (AM)
- Plasma-surface interactions (PSI)

$$\partial_{\parallel} \sim 0.01 \div 10^4 \quad m^{-1}$$

$$\partial_r \sim 10^2 \div 10^3 \quad m^{-1}$$

The SOL is extremely anisotropic!

Next generation machines (DEMO and fusion reactors) boundary plasma can be unmagnetized

SOL models (i): kinetic codes

First principle model – kinetic equation

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{\vec{F}}{m}\frac{\partial}{\partial \vec{V}}\right)f\left(\vec{r},\vec{V},t\right)=St$$

Neutral particles

$$\vec{F}=0,\quad St=St_B+St_{in}$$

$$St_B=\int u\sigma\left(f_a\left(\vec{V}_a{}'\right)f_b\left(\vec{V}_b{}'\right)-f_a\left(\vec{V}_a\right)f_b\left(\vec{V}_b\right)\right)d\vec{V}_a d\vec{V}_b\ ,$$

$$St_{in}=St_{in}^{+}-St_{in}^{-}$$

Plasma and impurity particles

$$\vec{F}=e\left(\vec{E}+\left[\vec{V}\times\vec{B}\right]\right),\quad St=St_{FK}+St_{in}+S_{wall}$$

$$St_{FP}^{a}=-\frac{\partial}{\partial \vec{V}}\sum_b \vec{A}(f_b)f_a\left(\vec{r},\vec{V},t\right)+\frac{\partial^2}{\partial\vec{V}\partial\vec{V}}\sum_b \vec{\vec{D}}(f_b)f_a\left(\vec{r},\vec{V},t\right)$$

$$S_{wall}=S_{wall}^{+}-S_{wall}^{-}$$

Dust particles

$$\vec{F}=e\left(\vec{E}+\left[\vec{V}\times\vec{B}\right]\right)+\vec{g}+\vec{R},\quad St=St_{dust-plasma}$$

$\vec{E}$ and $\vec{B}$

from Maxwell's system, or Ohms law (for *E*)

$$\nabla E=\frac{1}{\varepsilon_0}\rho\ ,\quad \nabla B=0$$

$$\nabla\times E=-\frac{\partial B}{\partial t}$$

$$\nabla\times B=\mu_0 j+\mu_0\varepsilon_0\frac{\partial E}{\partial t}$$

$$\Omega_e\tau_e>>1$$

$$E=\frac{j_\parallel}{\sigma_\parallel}+\frac{j_\perp}{\sigma_\perp}-V\times B+\frac{1}{en_e}\left(j\times B-\nabla p_e-0.71n_e\nabla T_e\right)$$

Direct simulation of particles

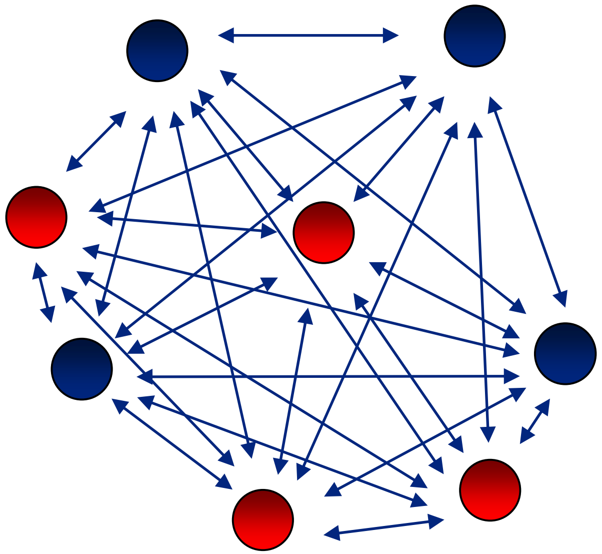
Particle-particle (PP) codes:

Number of operations to be performed on N particles scales as N^2.

First simulations: *Buneman 1959, Dowson 1962.* Simulation of 10^3 1D particles with direct resolution of Coulomb's interaction.

Today[1] **~ 10^8 particles** (MD modelling)

Too expensive for plasma simulations



8 particles – 57 interactions

Other possible options

- Direct solution of the Boltzmann equation
- Particle codes with Monte carlo collisions

PP can be excluded for neutral, impurity and plasma particle modelling in MCFP

[1] Jia, et al., [10.1109/SC41405.2020.00009](10.1109/SC41405.2020.00009)

Kinetic solvers for neutral particles

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}\right)f\left(\vec{r},\vec{V},t\right)=St_B+St_{in}+St_{wall}$$

$$St_h=\int u\sigma_h\left(f\left(\vec{V}_a'\right)f\left(\vec{V}_b'\right)-f\left(\vec{V}_a\right)f\left(\vec{V}_b\right)\right)d\vec{V}_a d\vec{V}_b\ ,$$
$$h=B,\ in\ \ (inelastic)$$

$$t,\ \vec{r},\ \vec{V}\rightarrow t_i,\ \vec{r}_{\vec{j}},\ \vec{V}_{\vec{k}}$$

100 meshes per dimention for r and V

Size of thew array of unknowns each time step $\mathbf{10^{2(D+V)}}$,

for 3D3V $\mathbf{10^{12}}$

Too large number!

Monte Carlo particle codes

1. Move particles $\dot{\vec{r}}=\vec{V}$
2. Calculate collision probability $P(t)=1-\exp(-\upsilon t),\quad \upsilon=nu\sigma(u)$
3. Collide particles, i.e. calculate after-collision velocities
4. Boundary conditions and sources (absorption, emission, ionization, etc.)

KE solver (probably!) can be excluded for neutral and impurity particle modelling in MCFP

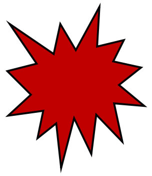
Collisions via Monte Carlo (MC) model

$P(t)$

$$P(t) = 1 - \exp(-\upsilon t)$$

$$\upsilon = n u \sigma(u)$$

Collision event



$$\begin{pmatrix} \vec{V}_1 \\ \vec{V}_2 \end{pmatrix} \Rightarrow \begin{pmatrix} \vec{V}_1' \\ \vec{V}_2' \end{pmatrix}$$

Equations conserving momentum and energy

i. Direct simulation MC

1. Calculation of average time between collisions $t_{col} = -\frac{\ln R}{\upsilon}, \quad R \in [0,1]$
2. Colliding particle after t_{col} time.

$\rightarrow$ $\mathbf{r}, \ \mathbf{V}, \ t_c$

ii. Null collision method

1. Calculation of shortest collision time $t_{col}^{\min} = -\frac{\ln R}{\upsilon_{\max}}$
2. Analyzing for collision after $t_{col}^{\min}$
3. Colliding these particles.

(e.g. **EIRENE**)

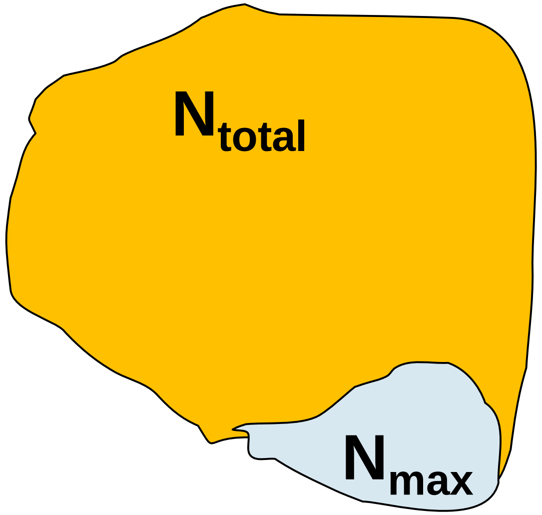
iii. Non-counter based model

1. Calculation of maximum number of collided particles

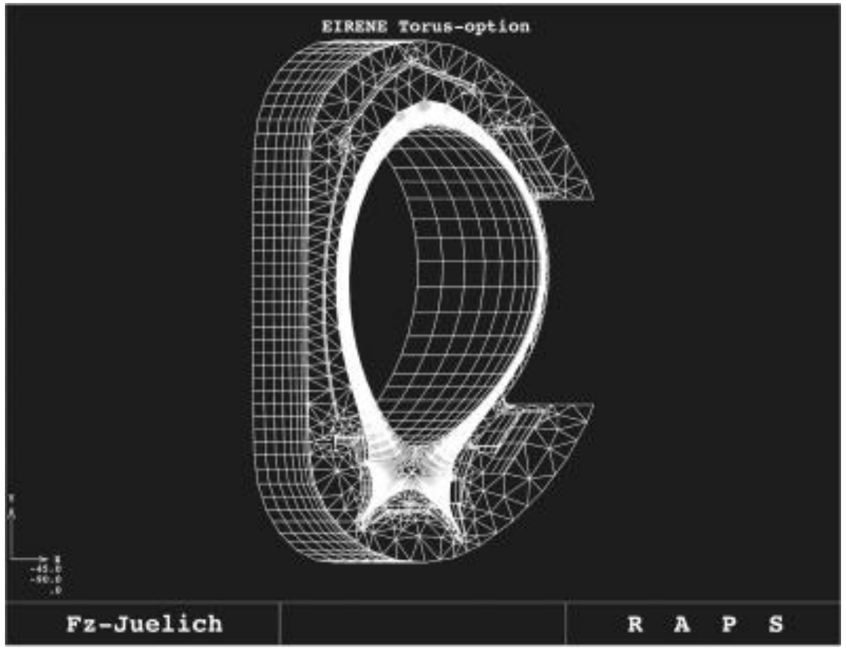
$$N_{\max} = N_{tot} P_{\max}(t) << N_{tot}$$

2. Analyzing for collision **only** N_{max} particles.
3. Colliding the selected particles.

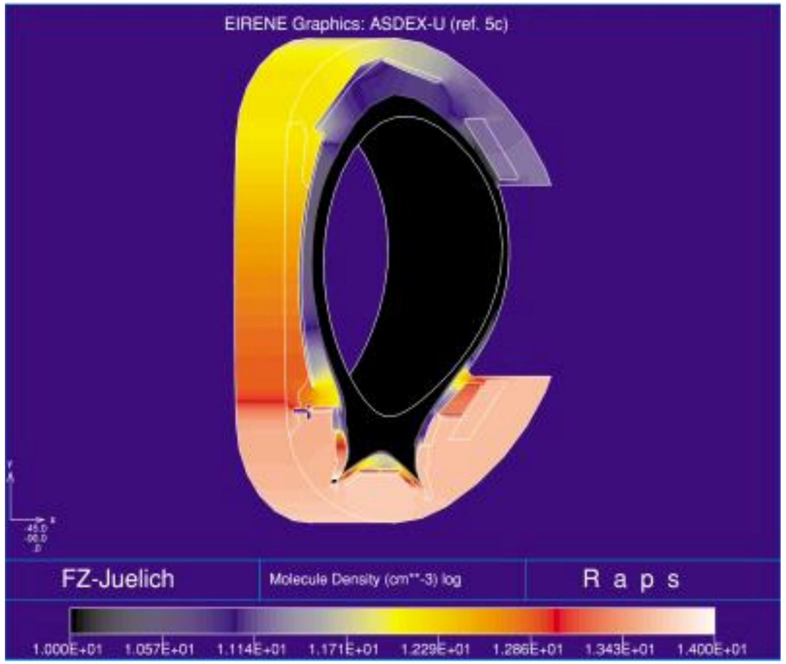
(e.g. **BIT-N**)



EIRENE[1]



EIRENE mesh for AUG[2].



Atomic density profiles fro EIRENE[2].

Limitation (of any MC)

For acceptable statistics very large number of simulation particles is required → heavy simulations

Questions?

[1][http://www.eirene.de]

[2][D. Reiter et al., FST 2005]

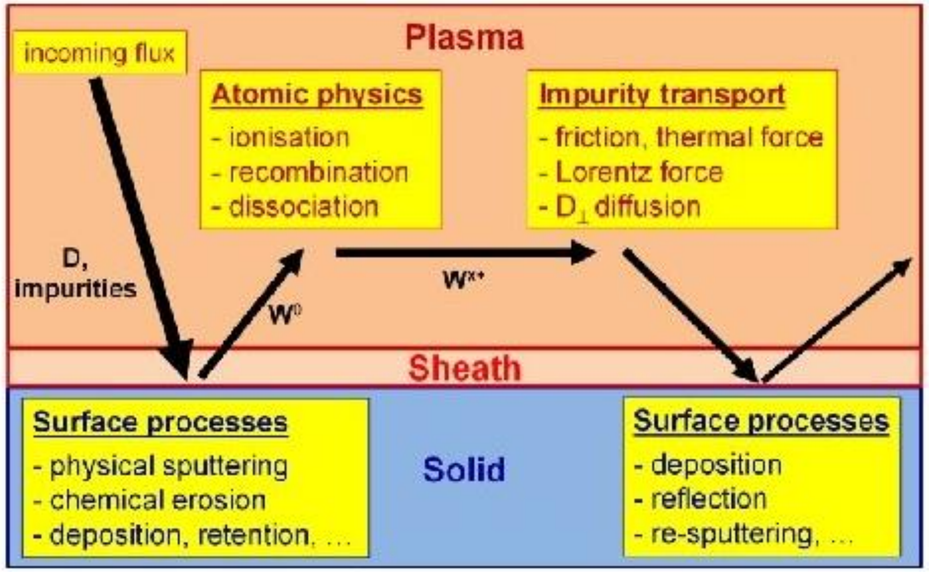
See the lecture 7 by F. Jaulmes/D. Tskhakaya

Impurity modelling

Two type of ions

- Main ions: H, D, T, He, ...
- Impurity ions, with much lower concentration

Impurity ions can pollute and cool down core and SOL plasmas



Simulation geometry of ERO (ERO-2)

Linear Monte Carlo (e.g. ERO)

Impurity particles interact with fluid/MHD plasma and wall

Advantage: relatively fast, Maxwell-averaged rate coefficients , R= <uσ>

Limitations: still slower than fluid models, **depends on plasma background** (to be provided)

$$\frac{d\vec{r}}{dt} = \vec{V}$$

$$\frac{d\vec{V}}{dt} = \frac{e}{m}\left(\vec{E} + \vec{V}\times\vec{B}\right) + \frac{1}{m}\vec{F}$$

Nonlinear Monte Carlo (PIC models, e.g. BIT-N)

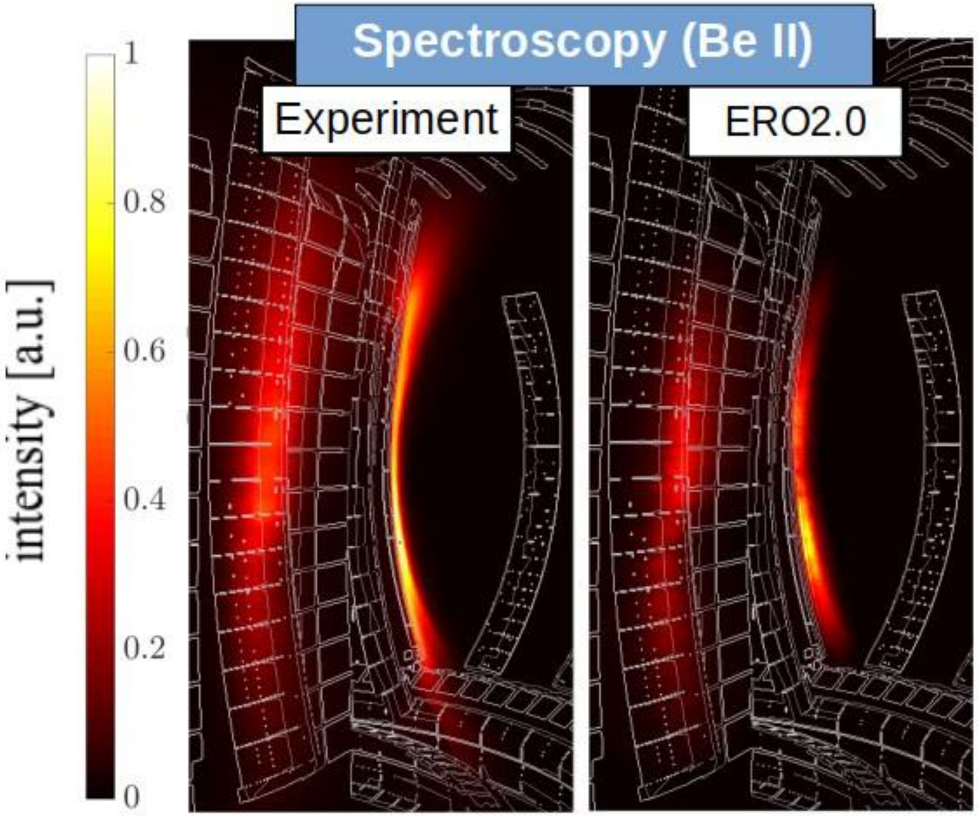
models including nonlinear interactions of impurity, neutral and plasma particles

Advantage: full kinetic treatment

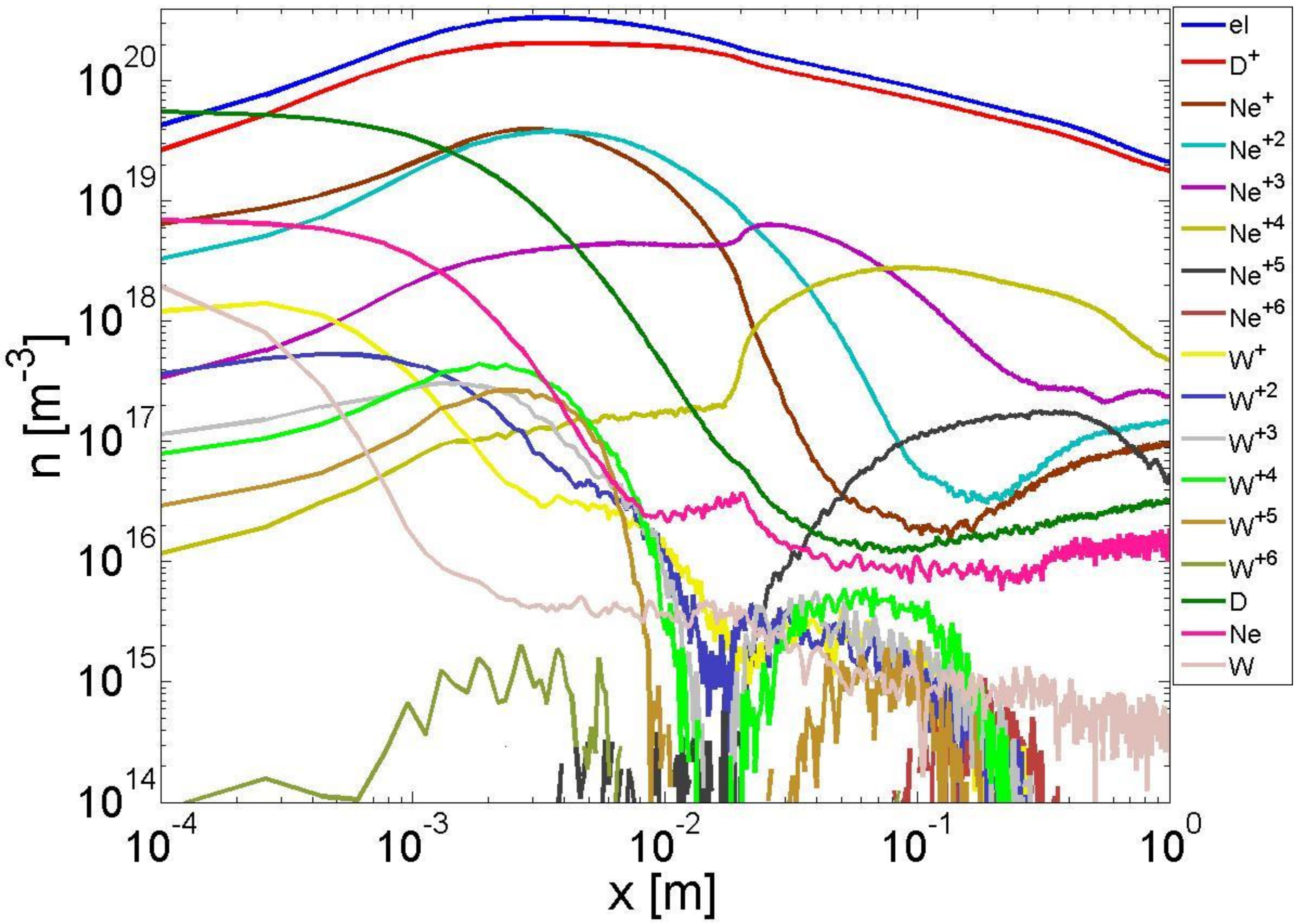
Limitations: **numerically very expensive**, exact cross-sections are required

Can be used for entire tokamak modelling!

Example of MC impurity transport codes



Be radiation profiles from experiment and ERO modelling [J. Romazanov et al., Phys. Scr. 2017]



Main and impurity particle profiles in the JET divertor plasma from BIT1 simulations [D. Tskhakaya, WP-PWIE 2023]

Kinetic modelling of the SOL plasmas

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{e}{m}\left(\vec{E}+\left[\vec{V}\times\vec{B}\right]\right)\frac{\partial}{\partial \vec{V}}\right)f\left(\vec{r},\vec{V},t\right)=St_{FK}+St_{in}+St_{wall}$$

Used for low dimensional problems

1D case $f_e(x, V, \mu)$, $\mu = V_{||}/V$, analytic solution[1]

$$\mu V\frac{\partial}{\partial x}f_e+\frac{e}{m_e}\frac{\partial\phi(x)}{\partial x}\left(\mu\frac{\partial}{\partial V}+\frac{1-\mu^2}{V}\frac{\partial}{\partial\mu}\right)f_e=\frac{\nu_{ei}}{2}\frac{\partial}{\partial\mu}\left(1-\mu^2\right)\frac{\partial}{\partial\mu}f_e$$

⇩

$$f_e(x,\mu,V)\approx f_M(x,V)+\mu\delta f(x,V),\quad |\delta f| << f_0$$

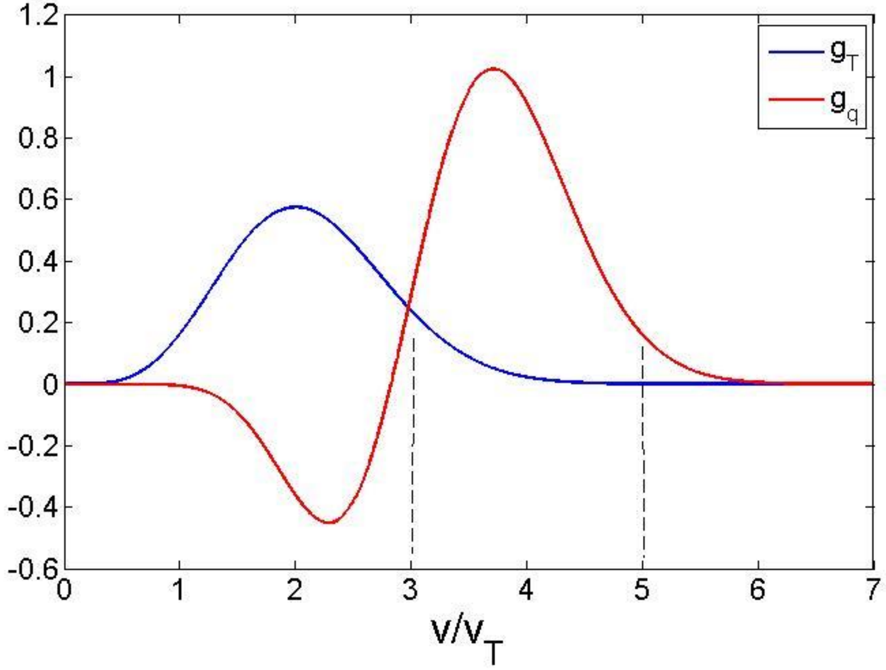
$$\delta f=\frac{-n_0}{\nu_{ei}(2\pi)^{3/2}V_T^2}\left(\frac{V}{V_T}\right)^4\left(\frac{V^2}{2V_T^2}-4\right)\exp\left(-\frac{V^2}{2V_T^2}\right)\frac{1}{T_e}\frac{\partial T_e}{\partial x},$$

⇩

$$T=T_e\int_0^\infty g_T(v)dv,\quad q_x=-\frac{2^7}{3\pi}\frac{n_0V_T^2}{\nu_{ee}}\frac{\partial}{\partial x}T_e\int_0^\infty g_q(v)dv$$

⇦

Required resolution > $V/5V_T$



[1] Chodura CPP 1992

PIC models of the plasma edge

Point particles

$$\frac{d\vec{r}}{dt} = \vec{V}$$

$$\frac{d\vec{V}}{dt} = \frac{e}{m}\left(\vec{E} + \vec{V} \times \vec{B}\right)$$

$$\rho, \vec{J}\ ?$$

Discretized space

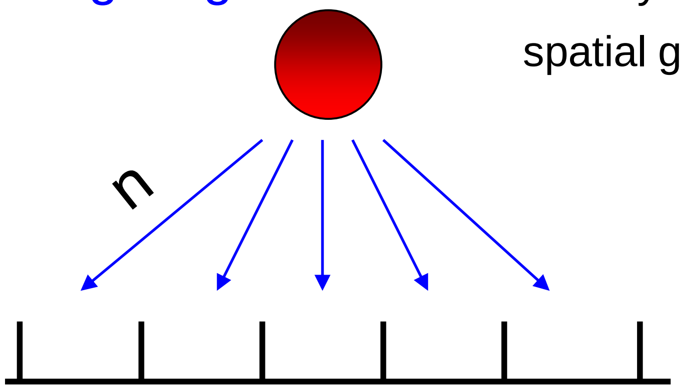
$$\nabla E = \frac{1}{\varepsilon_0}\rho \ , \quad \nabla B = 0$$

$$\nabla \times E = -\frac{\partial B}{\partial t}$$

$$\nabla \times B = \mu_0 j + \mu_0 \varepsilon_0 \frac{\partial E}{\partial t}$$

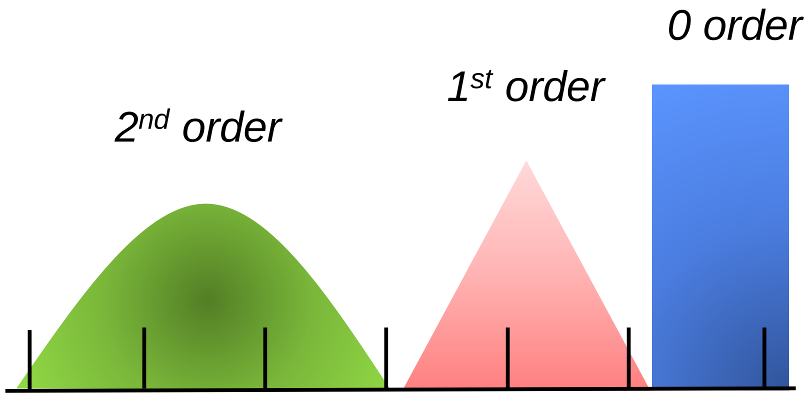
Particle weighting

assigning particle density to the spatial grids



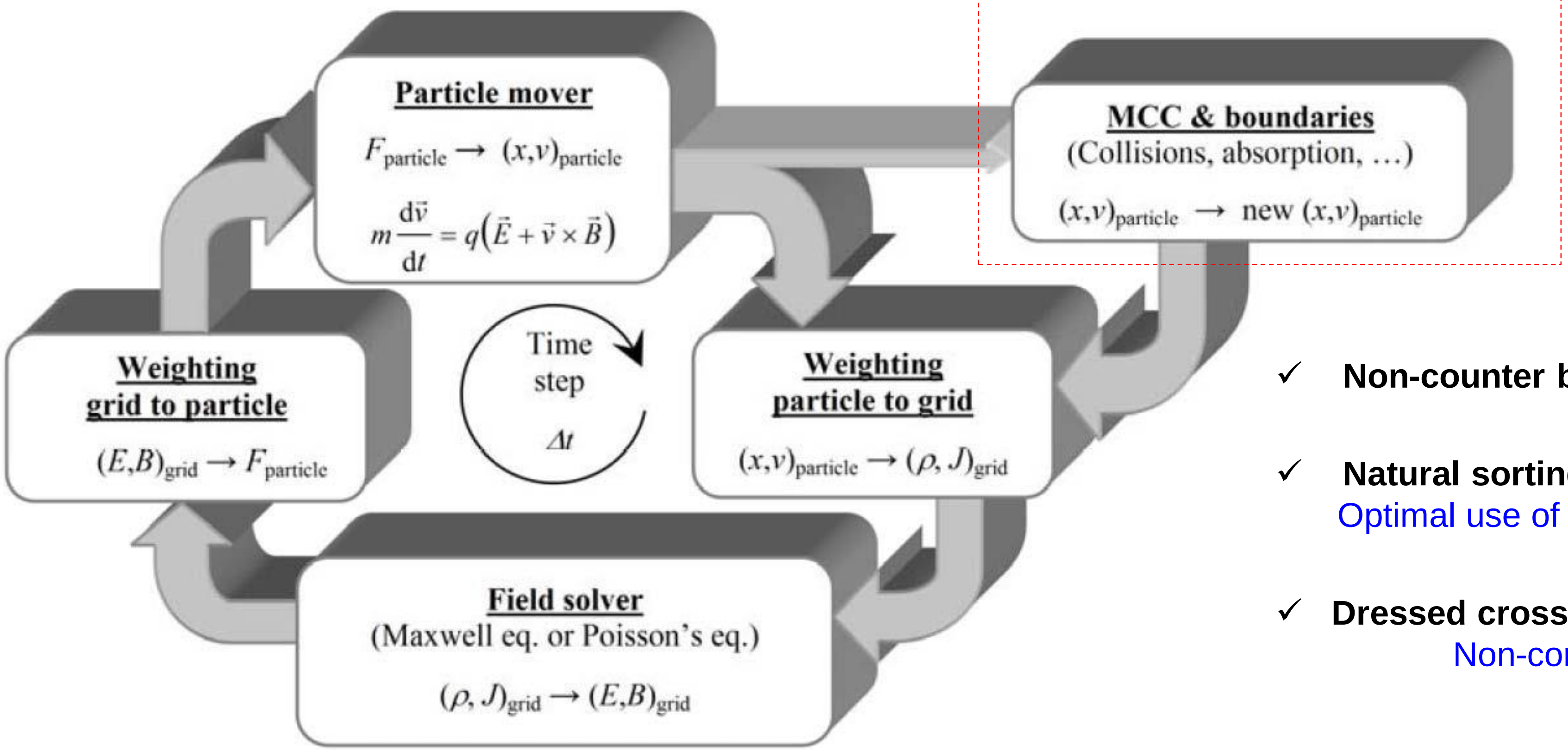
1D Grid cells

Different weighting schemes



Examples of full PIC + MC codes

1D3V (BIT1) and 3D3V (BIT3) electrostatic PIC + Monte Carlo



Specific for MCFP modelling

✓ **Non-counter based MC model**
fast, no limits on collision types

✓ **Natural sorting**
Optimal use of the cache hit, easy space decomposition, no limitation* on system size

✓ **Dressed cross section model**
Non-coronal approximation for high density plasmas

✓ **Physics based Poisson solver**
accurate, fast and highly scallable[1]

See the lecture 3 by D. Tskhakaya

On full PIC + MC models

Advantage

- Fully kinetic, compromises
- Easy to treat plasma-wall interactions
- Massive parallelization is straightforward

Limitation

- Requires extremely heavy simulation
- Numerical oscillations can lead to incorrect results (and crashes). Energy conservation diagnostic should be used
- Hard to find necessary collision cross-sections

Questions?

Drift kinetic models

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{e}{m}\left(\vec{E}+\left[\vec{V}\times\vec{B}\right]\right)\frac{\partial}{\partial \vec{V}}\right)f_a\left(\vec{r},\vec{V},t\right)=St^a_{FK}+St^a_{in}+St^a_{wall}$$

$$\rho=\frac{V_T}{\Omega}\to 0,\ \ \Omega=\frac{eB}{m} \quad \Rightarrow \quad \vec{V}=\vec{V}_{\parallel}+\vec{V}_{ExB},\quad \vec{V}_{ExB}=E\times B/B^2$$

$$\left(\frac{\partial}{\partial t}+\vec{V}_{\parallel}+\vec{V}_{ExB}\frac{\partial}{\partial \vec{r}}+\frac{e}{m}E_{\parallel}\frac{\partial}{\partial V_{\parallel}}\right)f_a\left(\vec{r},V_{\parallel},t\right)=St^a_{DK}$$

+ Field equations (e.g.): $\Delta\varphi=-\frac{\rho}{\varepsilon_0},\ \vec{E}=-\frac{\partial}{\partial\vec{r}}\varphi$

Advantage

- faster than Gyro-kinetic,
- Nonlinear drift-Fokker-Planck collision operator exists
- Can be used for core and edge plasmas

Limitations:

- still requires heavy simulation,
- all finite gyro-radius effects are neglected

Gyro-kinetic models

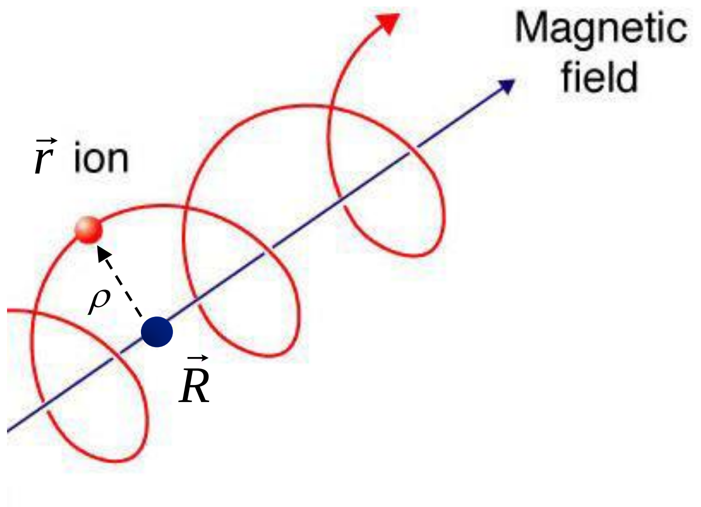
$$\vec{r} = \vec{R} + \cos(\Omega t)\vec{\rho}, \qquad \rho = \frac{V_T}{\Omega} << 1,$$ [1, 2]

$$\left(\frac{\partial}{\partial t} + \dot{\vec{R}} \frac{\partial}{\partial \vec{R}} + \dot{V}_{\parallel} \frac{\partial}{\partial V_{\parallel}} \right) f_a\left(\vec{R}, V_{\parallel}, \mu, t\right) = St^{a}_{FK,linear}$$

$$\dot{\vec{R}} = V_{\parallel}\vec{b} + \bar{\vec{E}} \times \vec{b} / B + \vec{b} \times \left(\frac{V_{\parallel}^2}{\Omega} \frac{\partial}{\partial R_{\parallel}} \vec{b} + \frac{\mu}{q} \frac{\partial}{\partial \vec{R}} \ln B \right)$$

$$\dot{V}_{\parallel} = \left(\frac{q}{m} \bar{\vec{E}} - \mu \frac{\partial}{\partial \vec{R}} B \right) \cdot \left(\vec{b} + \frac{V_{\parallel}}{\Omega} \vec{b} \times \frac{\partial}{\partial R_{\parallel}} \vec{b} \right)$$

$$\mu = \frac{m V_{\perp}^2}{2B}, \quad \bar{\vec{E}} = \oint \vec{E}(\vec{r}) d\theta / 2\pi$$



+ Field equations (simplified):

$$\Delta\varphi - \frac{\chi}{\lambda_D^2}(\varphi - \tilde{\varphi}) = -\frac{1}{\varepsilon_0}(\tilde{n}_i - n_e)$$

$$\tilde{n}_i(\vec{r}) = \int f_i(\vec{R}) \delta(\vec{R} - \vec{r} + \rho) B d\vec{R} d\theta dV_{\parallel} d\mu \neq n_i(\vec{r})$$

$$\tilde{\varphi}(\vec{r}) \neq \varphi(\vec{r})$$

[1] Lee, Phys. Fluids 1983
[2] Dubin et al., Phys. Fluids, 1983.

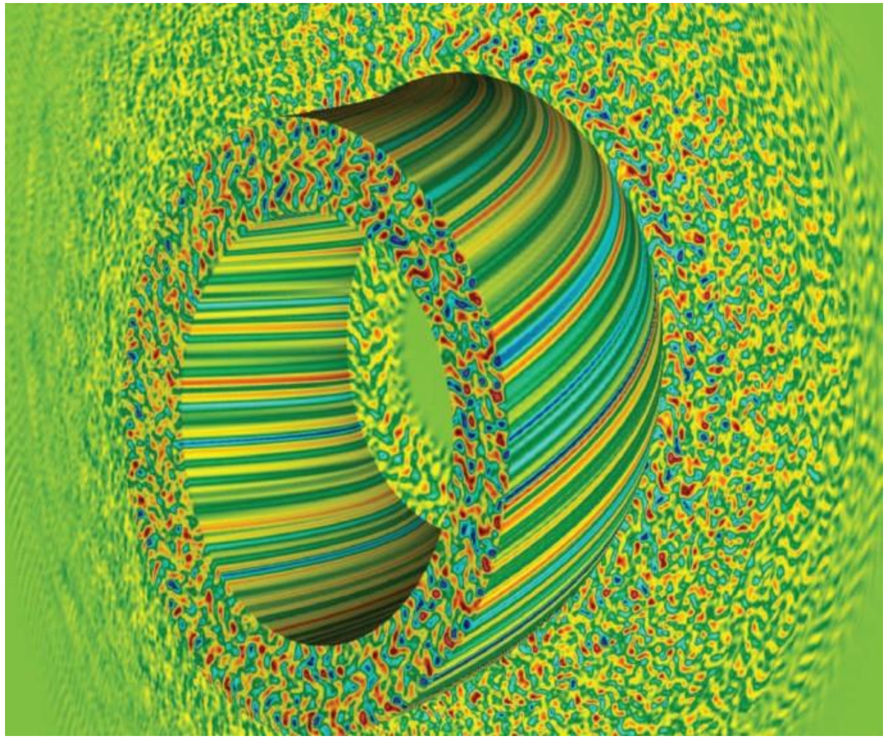
Gyro-kinetic models (ii)

Advantage

- golden compromise between the simulation speed and physics model
- finite gyro-radius effects are accounted
- Used for core and edge plasmas

Limitation

- requires heavy simulation,
- hard to implement collisions: majority use linear FP models, no interaction with other particles except ion + electron
- Could not „touch“ the wall
- Limited resolution (i.e. Number of V meshes)



Gyro-kinetic simulation of ITER plasmas[1]

Questions?

[1] Villard, et al., Plas. Phys. Cont. Fus. , 2013

Fluid models of the plasma edge

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{e}{m}\left(\vec{E}+\left[\vec{V}\times\vec{B}\right]\right)\frac{\partial}{\partial \vec{V}}\right)f\left(\vec{r},\vec{V},t\right)=\underline{St_{FK}+St_{in}+St_{wall}}$$

+ field equations (***E***, ***B***)

$$\times\int_{\vec{V}}\vec{V}^m d\vec{V}^{[1]}$$

$$\frac{\partial}{\partial t}A^m-\vec{\nabla}\vec{\Gamma}_A^m=S_A^m$$

$$A^0=n,\qquad A^1=n\vec{V},\ \ A^2=nT+\dots$$

$$\Gamma_n^0=n\vec{V},\ \dots\qquad S_n^0=n\left(\upsilon_{ion}-\upsilon_{rec}\right),\dots$$

$$\frac{\partial}{\partial t}n_s+\vec{\nabla}n_s\vec{V}_s=\sum_j \underline{S_{sj}}$$

$$S_{sj}=\int_{-\infty}^{+\infty}\underline{St_{in}^{sj}}d\vec{V},\quad \vec{R}_{sj}=m_s\int_{-\infty}^{+\infty}\left(St_{FP}^{sj}+\underline{St_{in}^{sj}}\right)\vec{V}d\vec{V},\quad \vec{Q}_{sj}=\frac{m_s}{2}=\int_{-\infty}^{+\infty}\left(St_{FP}^{sj}+\underline{St_{in}^{sj}}\right)V^2d\vec{V}$$

$$m_sn_s\left(\frac{\partial}{\partial t}\vec{V}_s+\vec{V}_s\vec{\nabla}\vec{V}_s\right)=e_sn_s\left(\vec{E}+\vec{V}_s\times\vec{B}\right)-\vec{\nabla}n_sT_s+\sum_j\underline{\vec{R}_{sj}}$$

$$\frac{3}{2}n_s\left(\frac{\partial}{\partial t}T_s+\vec{V}_s\vec{\nabla}T_s\right)=-n_sT_s\vec{\nabla}\vec{V}_s-\vec{\nabla}\vec{q}_s+\sum_j\underline{Q_{sj}}\dots$$

For a simple el.-ion plasmas

$$S_{ei}=0,\quad \vec{R}_{ei}\sim -n\vec{\nabla}T_e-m_en\upsilon_{ei}\left(\vec{V}_e-\vec{V}_i\right)$$

$$Q_{ei}\sim-\left(\vec{V}_e-\vec{V}_i\right)\vec{R}_{ei}-\frac{3m_e}{m_i}n\upsilon_{ei}\left(T_e-T_i\right)$$

[1] Braginskii, Rev. Plasma Phys., 1965

Examples of SOL fluid codes

SOLPS-ITER, EDGE2D, UEDGE, SOLEDGE, CORDIV, EMC3, **SOLF1D**

Particle conservation equation in SOLPS-ITER code

$$\frac{\partial n}{\partial t} + \frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{\sqrt{g}}{h_x} n \left(b_x V_\parallel + b_z V_\perp^{(0)}\right)\right) + \frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{\sqrt{g}}{h_y} n V_y^{(0)}\right) = \underline{S^n} \, ,$$

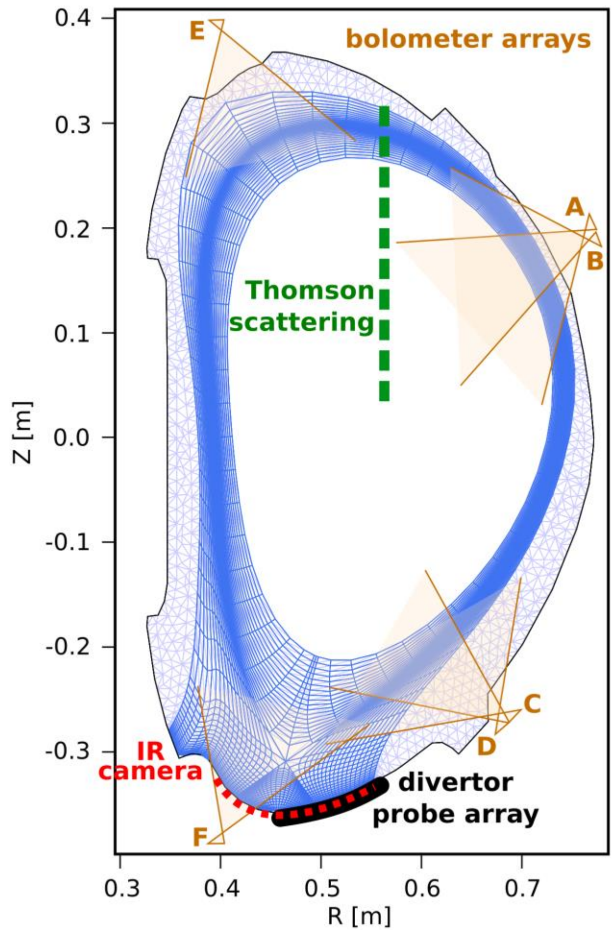
$$V_\perp^{(0)} = V_\perp^{(a)} + V_\perp^{(in)} + V_\perp^{(vis)} + V_\perp^{(s)} + \widetilde{V}_\perp^{(dia)} \, ,$$

$$V_y^{(0)} = V_y^{(a)} + V_y^{(in)} + V_y^{(vis)} + V_y^{(s)} + \widetilde{V}_y^{(dia)} \, ,$$

$$\widetilde{V}_\perp^{(dia)} = \frac{T_i B_z}{e b_z} \frac{\partial}{h_y \, \partial y}\left(\frac{1}{B^2}\right) \, ,$$

$$\widetilde{V}_y^{(dia)} = -\frac{T_i B_z}{e} \frac{\partial}{h_x \, \partial x}\left(\frac{1}{B^2}\right) \, .$$

The $h_{x,y}$ and g define the metric coefficients of the curvilinear coordinate system



SOLPS-ITER grid for COMPASS tokamak
[K. Hromasova, et al., EPS 2021]

„Static“ edge plasma fluid codes

Advantage

- fast
- Can model complex geometries
- Requires rate coefficients for atomic and PSI physics

Limitation

- Kinetic effects are neglected, or added ad hoc
- Neutrals are usually treated via separate (kinetic) MC codes
- Hard to treat multy-ion plasmas (there are new developments – Zhdanov‘s model)
- Slow time convergence

See the lecture 8 by I. Borodkina

Fluid turbulence codes

GBS –drift-reduced fluid code[1]

$$\frac{\partial n}{\partial t} = -\frac{\rho_\star^{-1}}{B}[\phi, n] + \frac{2}{B}[C(p_e) - nC(\phi)] - \nabla_\parallel(n v_{\parallel e}) + S_n$$

$$\frac{\partial \nabla_\perp^2 \phi}{\partial t} = -\frac{\rho_\star^{-1}}{B}[\phi, \nabla_\perp^2 \phi] - v_{\parallel i}\nabla_\parallel \nabla_\perp^2 \phi + \frac{B^2}{n}\nabla_\parallel j_\parallel + \frac{2B}{n}C(p)$$

$$\frac{\partial v_{\parallel e}}{\partial t} = -\frac{\rho_\star^{-1}}{B}[\phi, v_{\parallel e}] - v_{\parallel e}\nabla_\parallel v_{\parallel e} + \frac{m_i}{m_e}\left(\nu\frac{j_\parallel}{n} + \nabla_\parallel \phi - \frac{1}{n}\nabla_\parallel p_e - 0.71\nabla_\parallel T_e\right) + \frac{4}{3n}\frac{m_i}{m_e}\eta_{0,e}\nabla_\parallel^2 v_{\parallel e}$$

$$\frac{\partial v_{\parallel i}}{\partial t} = -\frac{\rho_\star^{-1}}{B}[\phi, v_{\parallel i}] - v_{\parallel i}\nabla_\parallel v_{\parallel i} - \frac{1}{n}\nabla_\parallel p + \frac{4}{3n}\eta_{0,i}\nabla_\parallel^2 v_{\parallel i}$$

$$\frac{\partial T_e}{\partial t} = -\frac{\rho_\star^{-1}}{B}[\phi, T_e] - v_{\parallel e}\nabla_\parallel T_e + \frac{4}{3}\frac{T_e}{B}\left[\frac{1}{n}C(p_e) + \frac{5}{2}C(T_e) - C(\phi)\right] + \frac{2}{3}T_e\left[0.71\nabla_\parallel j_\parallel - \nabla_\parallel v_{\parallel e}\right] + \chi_{\parallel,e}\nabla_\parallel^2 T_e + S_{T_e}$$

$$\frac{\partial T_i}{\partial t} = -\frac{\rho_\star^{-1}}{B}[\phi, T_i] - v_{\parallel i}\nabla_\parallel T_i + \frac{4}{3}\frac{T_i}{B}\left[C(T_e) + \frac{T_e}{n}C(n) - C(\phi)\right] + \frac{2}{3}T_i(v_{\parallel i} - v_{\parallel e})\frac{\nabla_\parallel n}{n} - \frac{2}{3}T_i\nabla_\parallel v_{\parallel e} - \frac{10}{3}\frac{T_i}{B}C(T_i) + \chi_{\parallel,i}\nabla_\parallel^2 T_i$$

$$[\phi, f] = \mathbf{b}\cdot(\nabla\phi \times \nabla f), \quad C(f) = B/2(\nabla\times \mathbf{b}/B)\cdot\nabla f, \quad \rho_\star = \rho_{s0}/R_0$$

Advantage

- Optimized for time-dependent problems
- Massively parallel
- Used for entire tokamak modeling

Limitation

- Reduced fluid equations
- Can model complex geometries

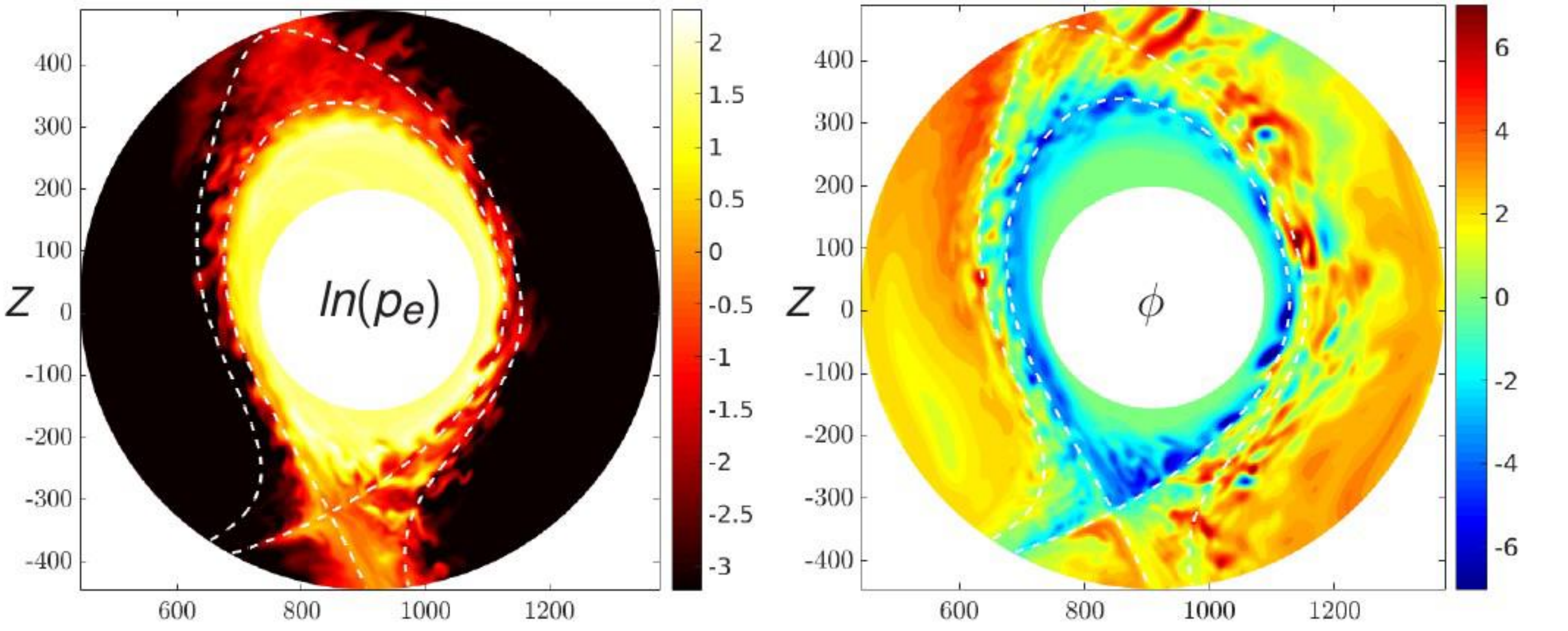
See the lecture by P. Macha

[1] Ricci et al., PPCF (2012)

Fluid turbulence code GBS (ii)

- GBS simulation run with:

$\rho_*^{-1} \sim 900$, $\chi_{\|e,i} = 1$, $\nu = 0.25$, ∇B drift points upwards



Used for core and edge plasmas

Questions?

From J. Horacek's lecture

1024 CPUs 4 months

MHD model

If we are interested in plasma motion as a single fluid → Magnetohydrodynamics (MHD)

$$\frac{\partial}{\partial t}n_s+\vec{\nabla}n_s\vec{V}_s=0,\quad s=e,i$$

$$m_s n_s\left(\frac{\partial}{\partial t}\vec{V}_s+\vec{V}_s\vec{\nabla}\vec{V}_s\right)=e_s n_s\left(\vec{E}+\vec{V}_s\times\vec{B}\right)-\vec{\nabla}n_sT_s+(\pm)\vec{R}_{ei}$$

$$n_e\approx n_i=n,\qquad p=n\left(T_e+T_i\right),$$

$$\rho=m_e n_e+M_i n_i\approx M_i n\qquad \vec{J}=en\left(\vec{V}_i-\vec{V}_e\right)$$

$$\vec{V}=\frac{m_e n_e\vec{V}_e+M_i n_i\vec{V}_i}{\rho}\approx\frac{m_e\vec{V}_e}{M}+\vec{V}_i\approx\vec{V}_i$$

$$(el)+(ion)$$

⬇

$$\frac{\partial}{\partial t}n+\vec{\nabla}n\vec{V}=0,$$

$$\rho\left(\frac{\partial}{\partial t}\vec{V}+\vec{V}\vec{\nabla}\vec{V}\right)=\vec{J}\times\vec{B}-\vec{\nabla}p$$

+ equation of state $\quad \frac{d}{dt}\frac{p}{\rho^{\gamma}}=0$

γ – adiabatic coefficient

MHD model (ii)

Full set of equations

$$\frac{\partial}{\partial t} n + \vec{\nabla} n \vec{V} = 0,$$

$$\rho\left(\frac{\partial}{\partial t}\vec{V} + \vec{V}\vec{\nabla}\vec{V}\right) = \vec{J} \times \vec{B} - \vec{\nabla} p$$

$$\frac{d}{dt}\frac{p}{\rho^{\gamma}} = 0$$

$$E + V \times B = \eta J$$

$$\nabla \times E = -\frac{\partial B}{\partial t}$$

$$\nabla \times B = \mu_0 j + \mu_0 \varepsilon_0 \frac{\partial E}{\partial t}$$

Low frequencies

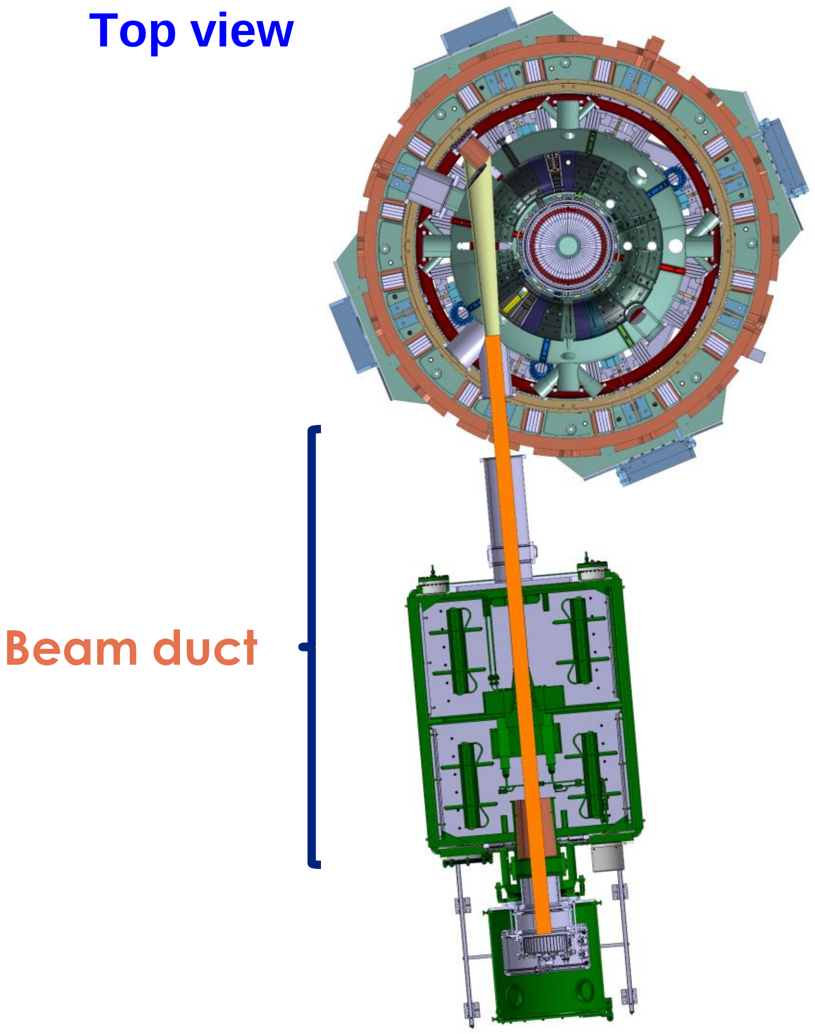
See the lecture 9 by A. Casolary/F. Jaulmes/P. Macha

Outline of the next lectures on MCFP

1. Feb 13 Introduction to modeling of laser-produced plasmas (LPP)– Limpouch
2. Feb 20 Introduction to different numerical methods used in Magnetic Confinement Fusion Plasmas (MCFP) - Tskhakaya
3. Feb 27 PIC for MCFP - Tskhakaya
4. Mar 6 Particle methods for LPP- Klimo
5. Mar 13 PIC simulations for extreme laser intensities – Jirka
6. Mar 20 Monte-Carlo methods for LPP- Klimo
7. Mar 27 MC modelling; examples used for plasma edge and for the NBI (Neutral Beam Injection) modelling - Tskhakaya, Jaulmes
8. Apr 3 Static fluid and Magnetohydrodynamics modelling of the MCFP – Borodkina, Jaulmes
9. Apr 17 Fluid transport modelling of the plasma core and edge - Jaulmes, Casolari, Mácha
10. Apr 24 Fluid simulations for LPP – Kuchařík
11. May 15 Atomic physics simulations – Limpouch
12. May 22 Machine learning methods - Seidl, Tomes

Introduction to Neutral Beam Injection (NBI) in tokamaks: fast ions modelling *[F. Jaulmes]*

- **What is the NBI [Neutral Beam Injector]**
- **Modelling particle orbits in tokamaks**
- **Overview of power deposition [COMPASS-U]**
- **Measurements & Modelling of fast neutrals generation in COMPASS**



Fluid modelling of the SOL (SOLPS-ITER)

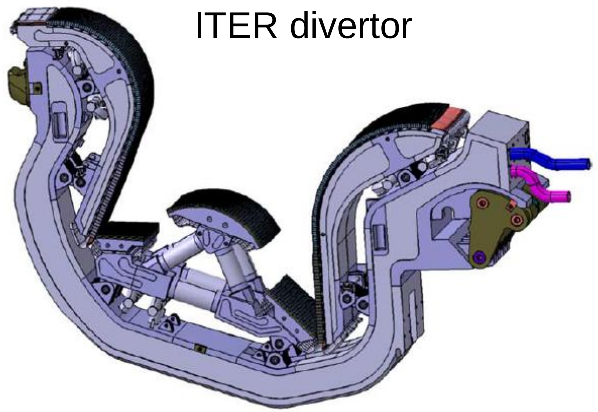
[I. Borodkina]

The SOLPS plasma boundary code package is dedicated to simulations of plasmas in the edge region of fusion devices:

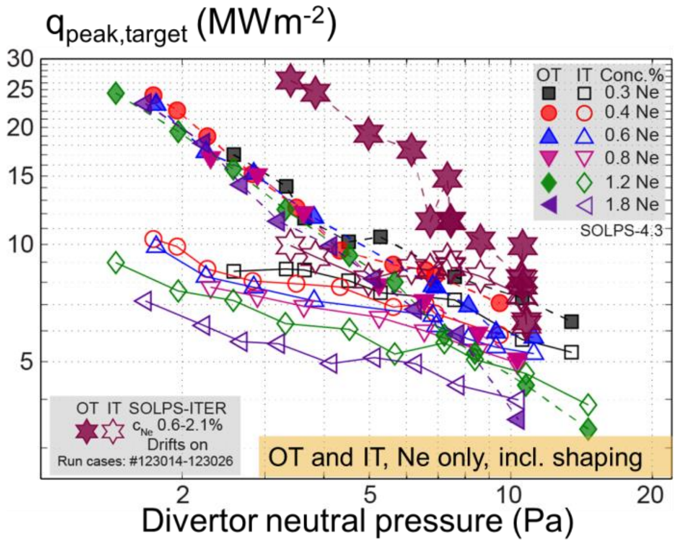
- **a 2D multi-fluid plasma (ions and electrons) transport code, B2**
- **and the 3D kinetic Monte Carlo neutral transport code EIRENE (accurate capture of neutral transport, account for the detailed wall interactions (pumping, fuelling) and wall geometry)**

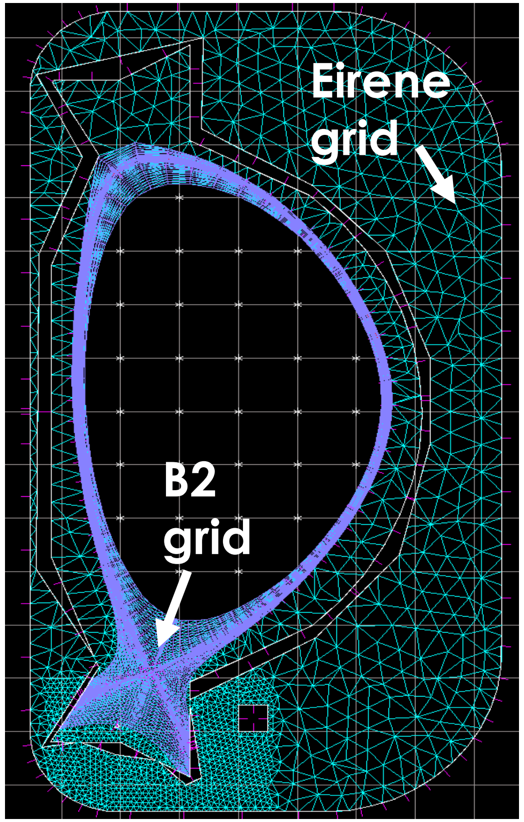
- **Maintained by ITER Organization at git.iter.org**
- **SOLSP-ITER successor SOLPS4.3 has been the main workhorse for the ITER divertor design studies since 20+ years**

ITER divertor



R.A. Pitts, et al, NME 2019



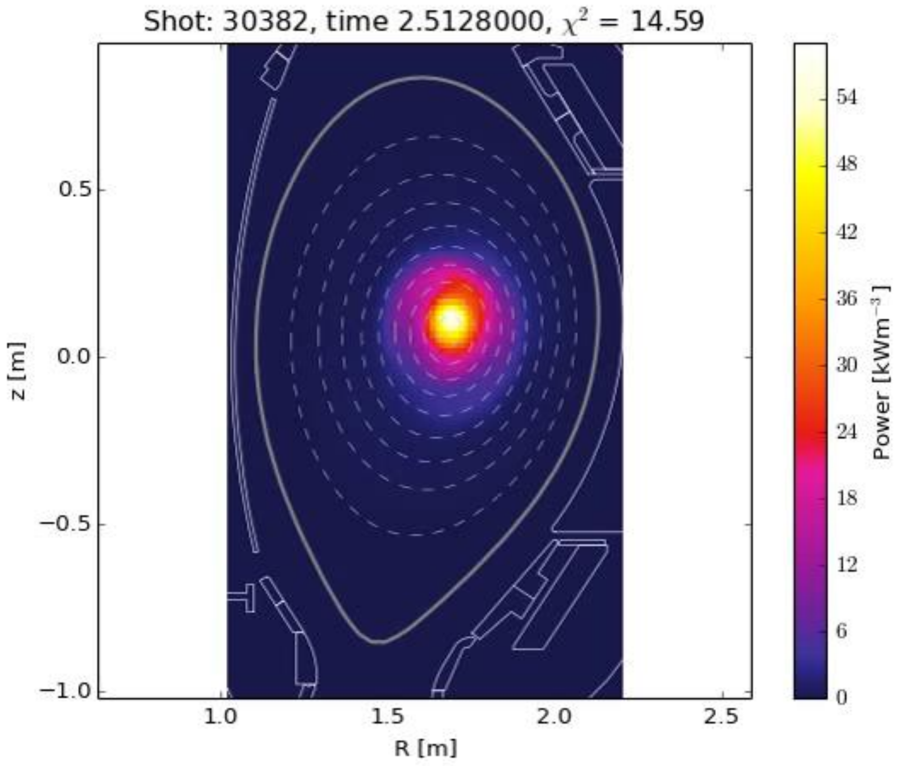


SOLPS-ITER grid (B2 and Eirene) for the COMPASS Upgrade tokamak developed in the IPP Prague

Introduction to the MHD modelling *[F. Jaulmes]*

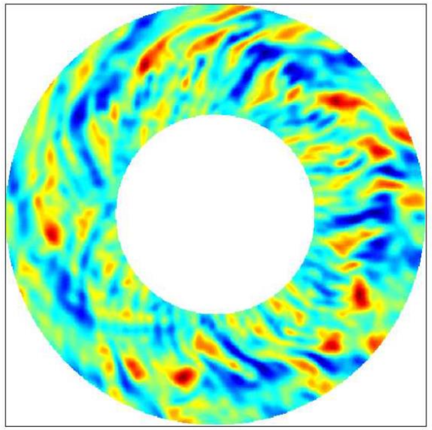
- **Safety factor profile in tokamaks**
- **Phenomenological description of MHD, the internal kink and the sawtooth crash**
- **Energy principle and derivation of linear growth rate**
- **Simplified poloidal mapping of the reconnecting magnetic flux & simplified Reconnection rate modelling [if time]**

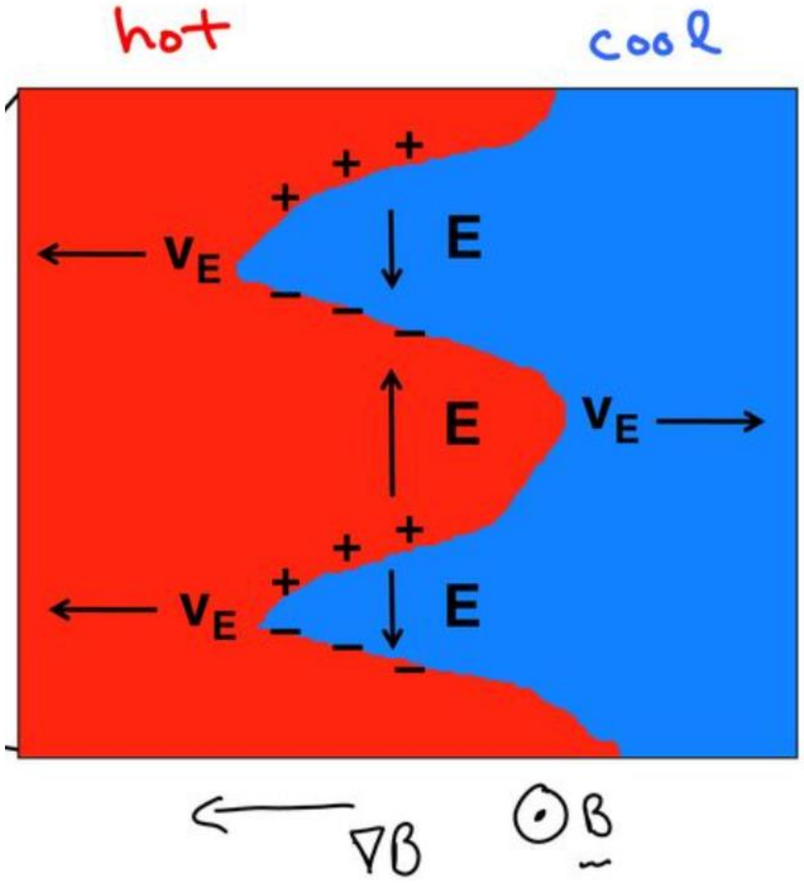
Sawtooth crash



Understanding micro-turbulence in a tokamak plasma

- **Principles of magnetic confinement and limitations of pressure gradients: particle and heat transport**
- **Derivation of numerical drift wave turbulence model in the edge of confined plasma**
- **Illustration: Edge Localized Modes**

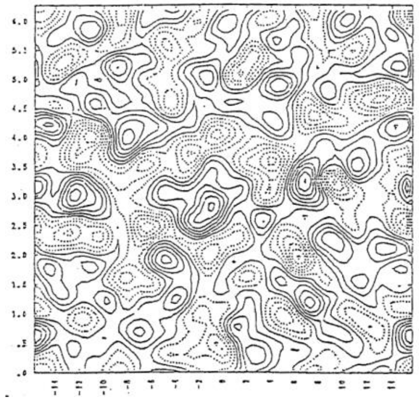


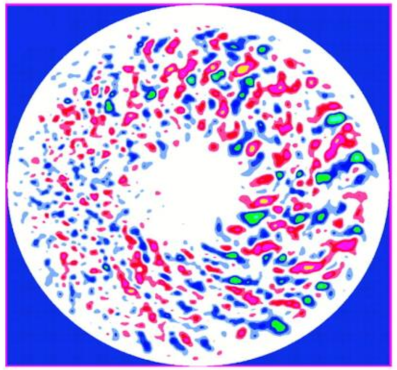


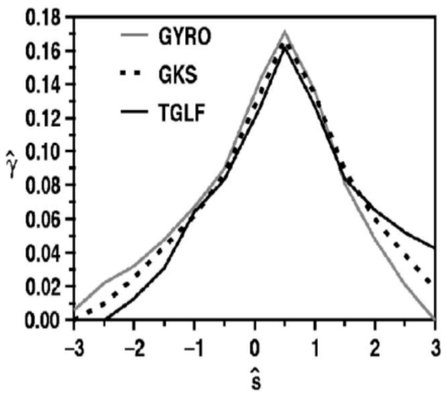
[P. Beyer, LPIIM]

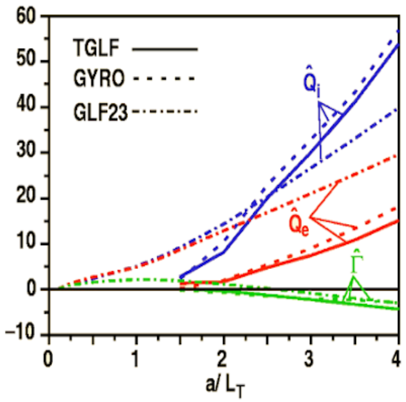
Introduction to gyro-fluid turbulence in tokamaks *[A. Casolari]*

- **Small-scale structures formation in turbulence (energy cascade, vortices)**
- **From single particle to fluid models**
- **From gyrokinetics to gyrofluid equations**
- **Gyro-Landau fluid (GLF) models**









Turbulence modelling of the SOL *[P. Macha]*

Perpendicular momentum:

$$\boldsymbol{v}_\perp = \overbrace{\frac{1}{B}\boldsymbol{b}\times\boldsymbol{\nabla}\phi}^{\text{ExB drift}} + \overbrace{\frac{1}{qnB}\boldsymbol{b}\times\boldsymbol{\nabla}p}^{\text{diamagnetic drift}} + \overbrace{\frac{m}{qB}\boldsymbol{b}\times\left(\frac{\partial}{\partial t}+\boldsymbol{v}\cdot\boldsymbol{\nabla}\right)\boldsymbol{v}}^{\text{polarization drift}},$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}_E = \overbrace{\boldsymbol{\nabla}\left(\frac{1}{B}\right)\cdot\boldsymbol{b}\times\boldsymbol{\nabla}\phi}^{(1)} + \overbrace{\frac{1}{B}\boldsymbol{\nabla}\times\boldsymbol{b}\cdot\boldsymbol{\nabla}\phi}^{(2)} = \mathcal{C}(\phi),$$

Kinetic equation

$$\frac{\partial f}{\partial t} + \nabla\cdot(vf) + \nabla\cdot\left(\frac{F}{m}f\right) = C$$

Density equation

$$\frac{\partial n}{\partial t} + \boldsymbol{\nabla}\cdot(n\boldsymbol{v}) = 0,$$

Temperature equation

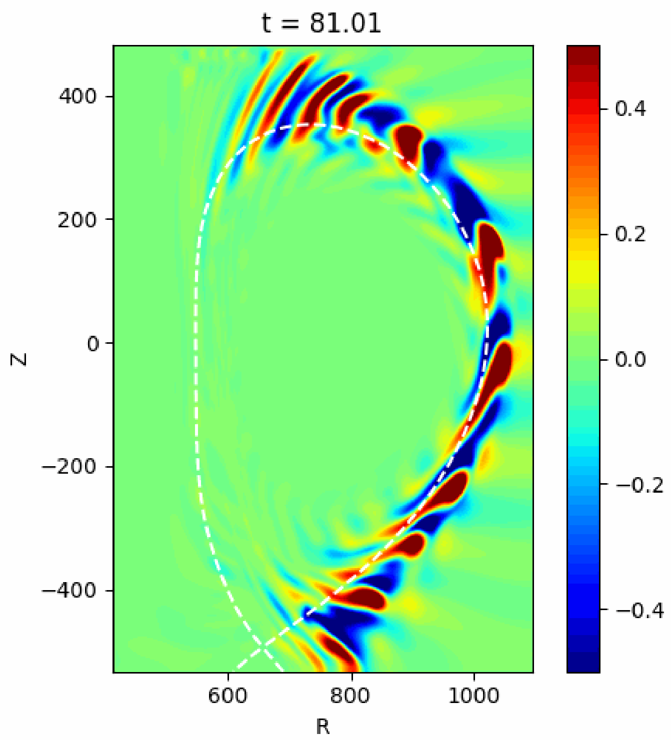
$$\frac{3}{2}n\left(\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla}\right)T + nT\boldsymbol{\nabla}\cdot\boldsymbol{v} + \boldsymbol{\nabla}\cdot\boldsymbol{q}_\perp = 0,$$

$$\begin{aligned}
\frac{\mathrm{d}n}{\mathrm{d}t} + n\mathcal{C}(\phi) - \mathcal{C}(nT) &= \Lambda(n)\\
\frac{\mathrm{d}T}{\mathrm{d}t} + \frac{2T}{3}\mathcal{C}(\phi) - \frac{7T}{3}\mathcal{C}(T) - \frac{2T^2}{3n}\mathcal{C}(n) &= \Lambda(T)\\
\frac{\mathrm{d}\Omega}{\mathrm{d}t} - \mathcal{C}(nT) &= \Lambda(\Omega)
\end{aligned}$$

$$\Omega = \boldsymbol{\nabla}\times v_E = B^{-2}\boldsymbol{\nabla}\times(\boldsymbol{B}\times\boldsymbol{\nabla}\phi) = \nabla_\perp^2\phi.$$

- from simple 2D model to complex 3D model
- Braginskii equations
- boundary conditions
- numerical implementation
- used schemes and solvers
- simulation results
- comparison with experiment
- advantages ╳ disadvantages

From simple 2D to complex 3D model



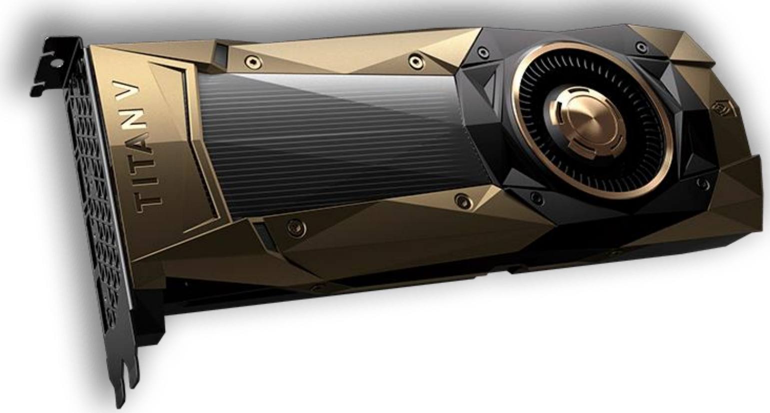
An example of density fluctuations during pre-quasi-stationary phase in GBS code.

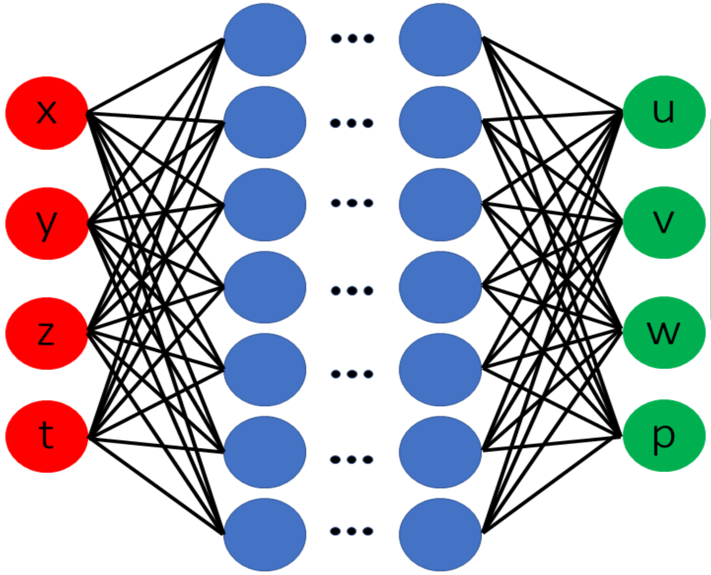
Python, GPU and Machine Learning

[J. Seidl and M. Tomes]

Covered topics

- Python for scientific computing and data science
- Speed up your simulations with GPU
- Autograd - automatic differentiation of computations
- What are Artificial Neural Networks (NN)
- Implicit representation of functions with NN
- Physics Informed Neural Networks - solving PDEs using NN





Naviers-Stokes loss

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}+\frac{\partial P}{\partial x}-\frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)=0$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}+\frac{\partial P}{\partial y}-\frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)=0$$

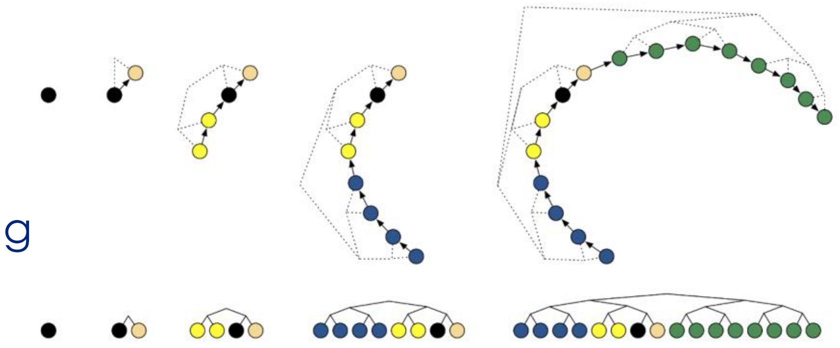
$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}+\frac{\partial P}{\partial z}-\frac{1}{Re}\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)=0$$

Experimental data loss

$$\|\vec{\mathbf{V}}-\vec{\mathbf{V}}_{\boldsymbol{exp}}\|^2=0$$

Bayesian Statistics *[J. Seidl and M. Tomes]*

- **P**robabilistic **P**rogramming **L**anguages
  - based on ML frameworks
  - utilise autograd, GPU speedups
- **Natural way of problem solving**:
  - What are the best parameters given a model and a priori knowledg
- Universal uncertainty propagation
- Optimisation algorithms: Hamiltonian samplers, NUTS
- Monte-Carlo Markov-Chain sampling



Bayesian Statistics