KNOSOS, a fast neoclassical code for three-dimensional magnetic configurations

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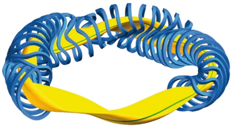
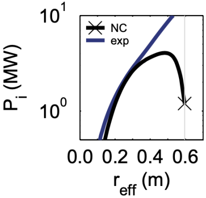
Motivation

Stellarators: intrinsically three-dimensional configurations.

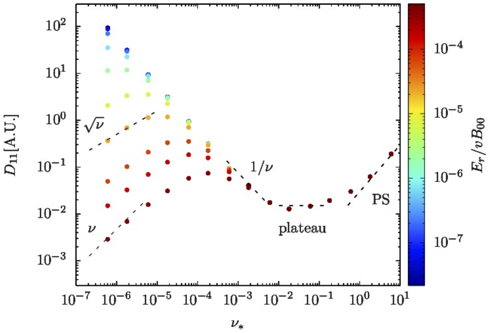




- Collisions + inhomogeneity of the magnetic field drive neoclassical transport that is very **different from the one in axisymmetric tokamaks**.
- **Relevant contribution to energy fluxes** in the core of reactor-relevant plasmas, even larger than turbulence, e.g. [Dinklage, NF (2013)].
- Configuration **optimized** with respect to neoclassical transport, crucial for achieving best performance of Wendelstein 7-X, e.g. [Beidler, submitted to Nature].
- **This talk:** neoclassical calculations of radial transport with the novel code `KNOSOS` (KiNetic Orbit-averaging SOlver for Stellarators).
  - **More efficient stellarator optimization.**
  - **Improved transport analyses.**

General goal: fast and accurate calculation of neoclassical transport at low collisionality

Radial transport in several **neoclassical regimes** as calculated with standard codes like DKES [Hirshman, PoF (1986)] (overview in [Beidler, NF (2011)]):



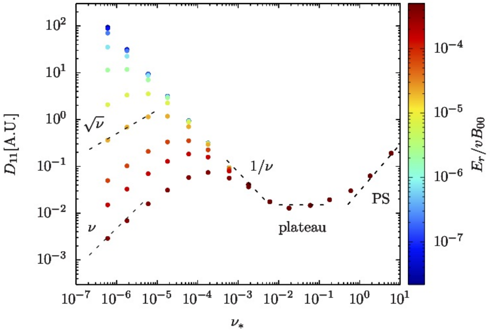
- At high collisionality, same as in axisymmetric tokamaks:
  - Pfirsch-Schlueter and plateau.
  - Numerical calculation is fast.
- At low collisionality, stellarator-specific regimes. For *standard* values of E_r:
  - $\epsilon^{3/2} \gg \nu_* \gg \rho_*/\epsilon \Rightarrow$ $1/\nu$ regime.
  - $\nu_* \ll \rho_*/\epsilon \Rightarrow \sqrt{\nu}$ or ν.

($\rho_* = \rho/R$ is the normalized Larmor radius, $\nu_* = R\nu/(\iota v)$ the collisionality, $\epsilon = a/R$ the inverse aspect ratio)

For small ν_* and large E_r, the piece of distribution function that is important for transport becomes increasingly localized in phase space $\Rightarrow$ **large computational cost**.

Goal I: **fast** and accurate calculation of neoclassical transport at low ν_* and E_r **of standard size**

The $1/\nu$ flux can be computed fast with the code `NEO` [Nemov, PoP (2007)], but no equivalently fast code exists for the $\sqrt{\nu}$ and ν regimes for arbitrary stellarator geometry.



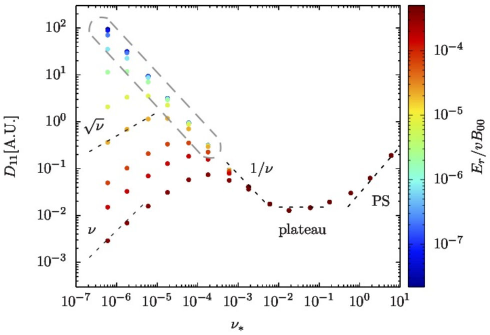
For this reason, stellarator optimization targets (successfully) the $1/\nu$ flux, e.g. [Beidler, submitted to Nature]:

- Transport of electrons (that are in the $1/\nu$ regime) is reduced.
- This causes negative E_r that indirectly reduces transport of ions (that are in the $\sqrt{\nu}$ or ν regimes).

Addressing directly the $\sqrt{\nu}$ **or** ν **flux** as well could lead to more efficient optimization. This requires a fast code and could be beneficial when additional optimization criteria (MHD, turbulence...) exist.

Goal II: fast and **accurate** calculation of neoclassical transport at low ν_* and **small** E_r

The component of the magnetic drift that is tangent to the flux-surface is typically ignored in the particle orbits.



This is accurate if

- the aspect ratio $1/\epsilon$ is large and,
- E_r has the standard size $\sim T_i/(a Z_i e)$.

But there are other scenarios:

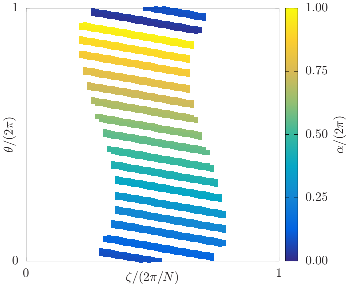
- compact stellarators (down to $1/\epsilon = 2.5$ [Ku, FST (2007)]), or
- small E_r (close to zero at the crossover between core $E_r > 0$ and $E_r < 0$, e.g. [Pablant, PoP (2018)]).

In these situations, for $\nu_* \ll \rho_*$, an additional regime may appear: **superbanana-plateau** (instead of the $1/\nu$ seen by `DKES`).

Coordinates on phase space

Spatial coordinates:

- $\psi = |\Psi_t|$ is the radial coordinate.
  - $2\pi\Psi_t$ is the toroidal magnetic flux.
- $\alpha = \theta - \iota\zeta$ labels magnetic field lines on the surface.
  - θ and ζ are Boozer angles and ι is the rotational transform.
- l is the arc length along the magnetic field line.



Velocity coordinates:

- $v = |\mathbf{v}|$ is the particle velocity.
- $\lambda = v_\perp^2/(v^2 B)$ is the pitch-angle coordinate.
- $\sigma = v_\|/v$ is the sign of the parallel velocity.

$$\begin{aligned}\mathbf{B} &= \Psi_t' \nabla\psi \times \nabla\alpha\,,\\ v_\| &= \mathbf{v}\cdot\mathbf{B}/B\,,\\ v_\perp &= \sqrt{v^2 - v_\|^2}\,.\end{aligned}$$

For each species b: compute the deviation of the distribution function from a Maxwellian $F_{M,b}$ for *trapped particles*, $g_b(\psi, \alpha, \lambda, v)$.

Drift kinetic equation

$$\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\||} \left(\mathbf{v}_{M,b} + \frac{B}{\langle B \rangle} \mathbf{v}_E \right) \cdot \nabla\alpha \left(\partial_\alpha + \partial_\alpha \lambda|_J \partial_\lambda \right) g_b - \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\||} C_b^{\mathrm{lin}}[g_b] =$$

$$= - \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\||} (\mathbf{v}_{M,b} + \mathbf{v}_E) \cdot \nabla\psi \Upsilon_b F_{M,b} \, .$$

At boundary between trapping and passing particles, $g_b = 0$. Here:

- Coefficients of the equation: integrals over l between bounce points l_{b_1} and l_{b_2} (where $v_\| = 0$):
$$\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\||} (\ldots) = \frac{1}{v} \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{\sqrt{1 - \lambda B(\alpha, l)}} (\ldots) \, .$$
- $C_b^{\mathrm{lin}}[g_b] = \frac{\nu_{\lambda,b} v_{||}}{v^2 B} \partial_\lambda \left(v_{||} \lambda \partial_\lambda g_b \right)$ is the linearized pitch-angle collision operator.
- $\Upsilon_b = \frac{\partial_\psi F_{M,b}}{F_{M,b}} = \frac{\partial_\psi n_b}{n_b} + \frac{\partial_\psi T_b}{T_b} \left(\frac{m_b v^2}{2 T_b} - \frac{3}{2} \right) + \frac{Z_b e \partial_\psi \varphi_0}{T_b}$ is a combination of thermodynamical forces.
- $\mathbf{v}_{M,b} = \frac{m_b v^2}{Z_b e} \left(1 - \frac{\lambda B}{2} \right) \frac{\mathbf{B} \times \nabla B}{B^3}$ and $\mathbf{v}_E = - \frac{\nabla \varphi \times \mathbf{B}}{B^2}$ are the magnetic and $E \times B$ drifts.
- $\varphi(\psi, \alpha, l) = \varphi_0(\psi) + \varphi_1(\psi, \alpha, l)$, with $|\varphi_1| \ll |\varphi_0|$.
- The term with $\partial_\alpha \lambda|_J \equiv - \left(\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\||} \lambda \partial_\alpha B \right) / \left(\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\||} B \right)$ ensures conservation of J.

Assumptions (details in [Calvo (2017) PPCF, d'Herbemont (in preparation)])

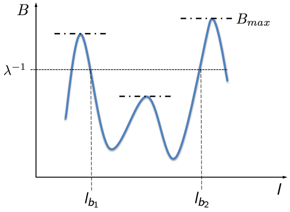
At low collisionality, **motion of trapped particles along B** (i.e. in l) **much faster than collisions**.

$\Rightarrow$ Distribution function independent of arc-length l.

$\Rightarrow$ Coefficients of the equation: integrals over l between bounce points:

$\Rightarrow$ Differential equation in two variables: λ and α.

$\Rightarrow$ Fast computation.



Common to most codes: in order to describe neoclassical transport with a **radially local** equation (instead of a global code such as `FORTEC-3D` [Satake (2008), PFR]) the magnetic configuration needs to

- have large aspect-ratio* [d'Herbemont (in preparation)] and/or

  (* this also allows to use the pitch-angle collision operator)

- be close to omnigeneity, i.e., to perfect neocl. optimization [Calvo (2017) PPCF].

As a result of this, our radially-local bounce-averaged equation is valid in two limits, corresponding to the two calculations that we will present next.

Drift kinetic equation in the limit of large-aspect ratio

In this section, $\epsilon \ll 1$ and $E_r \sim T/(a\,Ze)$. Therefore, in equation

$$\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\parallel|}\left(\mathbf{v}_{M,b} + \frac{B}{\langle B\rangle}\mathbf{v}_E\right)\cdot\nabla\alpha\,(\partial_\alpha + \partial_\alpha\lambda|_J\partial_\lambda)\,g_b - \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\parallel|} C_b^{\mathrm{lin}}[g_b] =$$

$$= -\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\parallel|}(\mathbf{v}_{M,b} + \mathbf{v}_E)\cdot\nabla\psi\Upsilon_b F_{M,b}\,,$$

the terms $\mathbf{v}_{M,b}\cdot\nabla\alpha$ and $\mathbf{v}_E\cdot\nabla\psi$ terms are negligible. We are left with

$$\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\parallel|}\frac{B}{\langle B\rangle}\mathbf{v}_E\cdot\nabla\alpha\,(\partial_\alpha + \partial_\alpha\lambda|_J\partial_\lambda)\,g_b - \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\parallel|} C_b^{\mathrm{lin}}[g_b] = -\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\parallel|}\mathbf{v}_{M,b}\cdot\nabla\psi\Upsilon_b F_{M,b}\,.$$

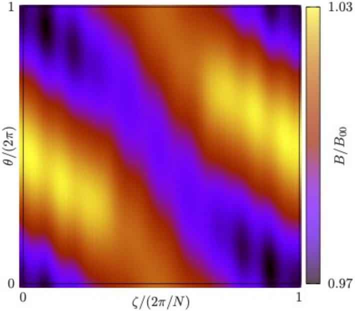
This equation models rigorously the transport of large aspect-ratio stellarators at low collisionality [d'Herbemont (in preparation)]. Specifically, it describes:

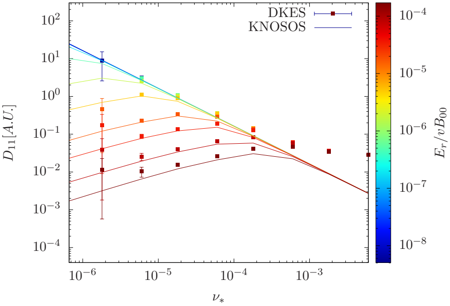
- $\epsilon^{3/2} \gg \nu_* \gg \rho_*/\epsilon \Rightarrow 1/\nu$ regime.
- $\nu_* \ll \rho_*/\epsilon \Rightarrow \sqrt{\nu}$ or ν regimes.

For large aspect ratio, this equation coincides with the orbit average of the equation solved by DKES.

Monoenergetic transport coefficient in the $1/\nu$ and $\sqrt{\nu}$ regimes: comparison between KNOSOS vs. DKES

- Calculate D_{11} as a function of $s=\frac{\psi}{\psi_{LCMS}}$, ν_* and $\frac{E_r}{vB_{00}}$, with $Q_b \sim \int \mathrm{d}v F_{M,b}\Upsilon_b D_{11}$.
- W7-X low-mirror (AIM), $s=0.046$ *(other devices at [Velasco, JCP (2020)])*





- Overall good agreement.
- Calculation of a flux-surface takes **seconds in a single processor** (instead of hours).
  - Fast enough to be included in a stellarator optimization suite.

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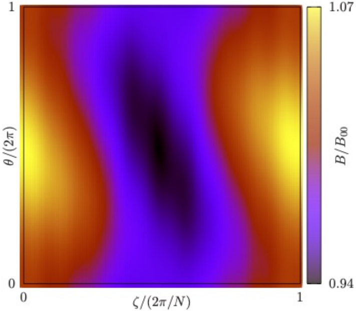

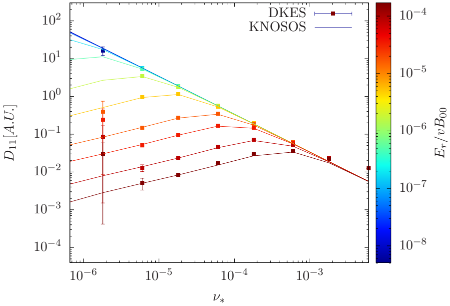

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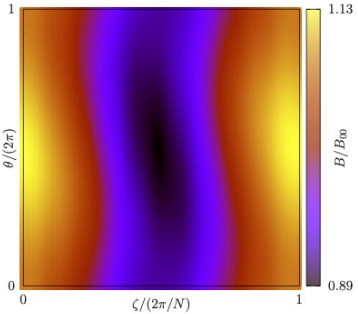

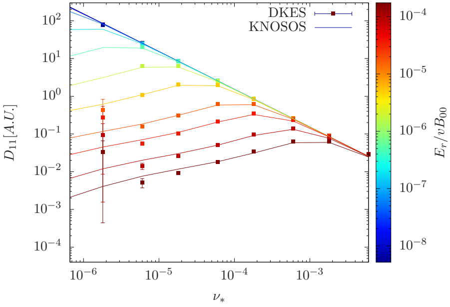

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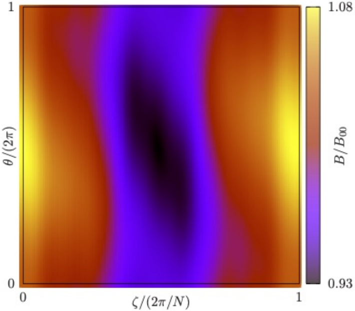

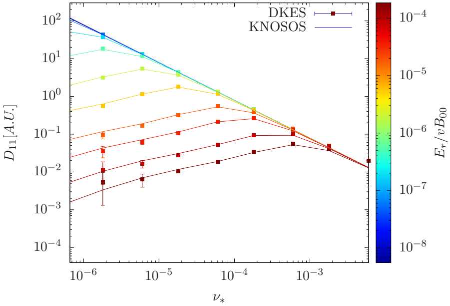

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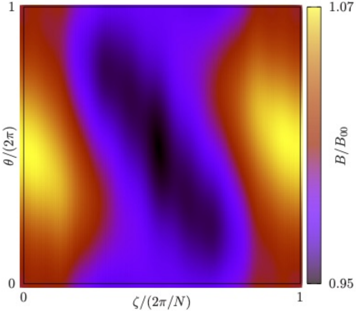

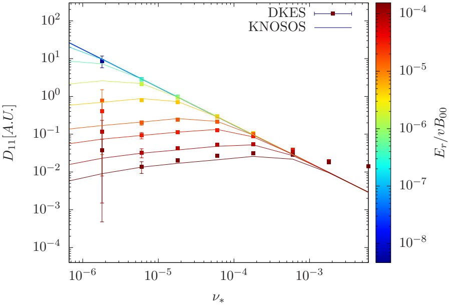

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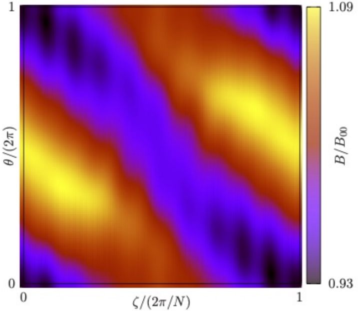

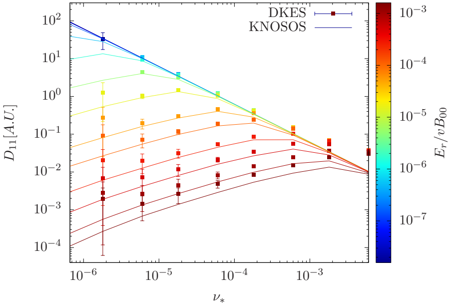

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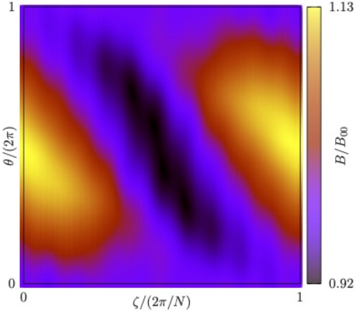

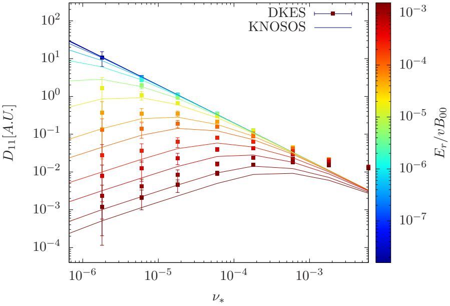

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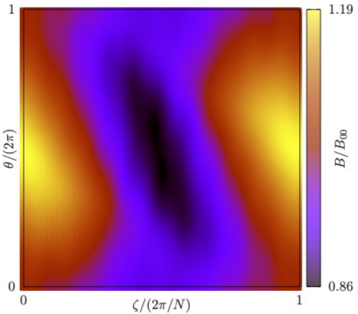

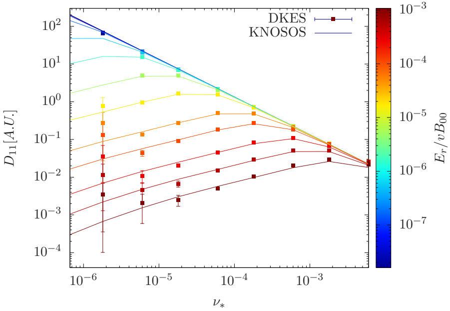

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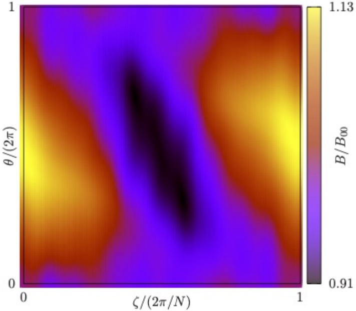

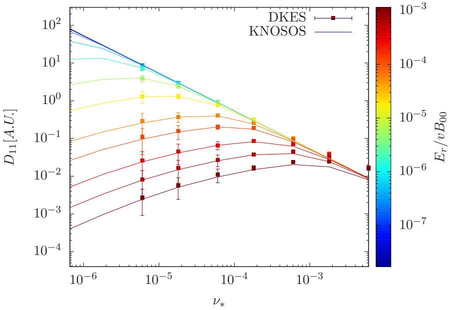

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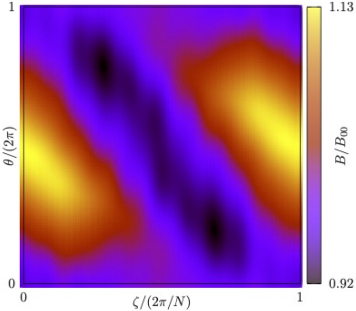

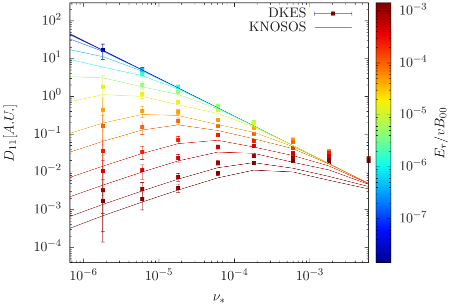

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Drift kinetic equation for small E_r in optimized stellarators

In this section, $\epsilon \ll 1$ **but** $E_r \ll T/(a\,Ze)$. Therefore, in equation

$$\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\|\|} \left(\mathbf{v}_{M,b} + \frac{B}{\langle B\rangle}\mathbf{v}_E\right) \cdot \nabla\alpha \left(\partial_\alpha + \partial_\alpha\lambda|_J\partial_\lambda\right) g_b - \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\|\|} C_b^{\mathrm{lin}}[g_b] =$$

$$= - \int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{|v_\|\|} (\mathbf{v}_{M,b} + \mathbf{v}_E) \cdot \nabla\psi \Upsilon_b F_{M,b}\,,$$

the terms $\mathbf{v}_{M,b} \cdot \nabla\alpha$ and $\mathbf{v}_E \cdot \nabla\psi$ are not negligible [Calvo (2017) PPCF]:

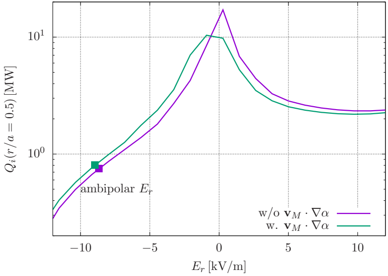
- The term $\partial_\alpha\lambda|_J\partial_\lambda$ is small in this limit, but we retain it in order to deal numerically with very deeply trapped particles [Velasco (2020) JCP].

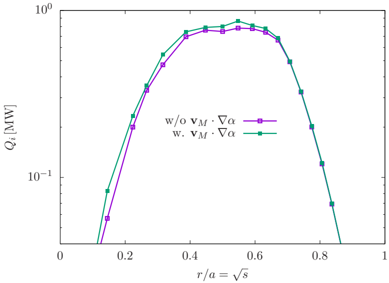
This equation models rigorously the transport of optimized large-aspect ratio stellarators at low collisionality [Velasco (2020) JCP]. Specifically, for small E_r, it describes:

- $\epsilon^{3/2} \gg \nu_* \gg \rho_* \Rightarrow 1/\nu$ regime.
- $\nu_* \ll \rho_* \Rightarrow$ superbanana-plateau or $\sqrt{\nu}$ regimes.

Relevance of the tangential magnetic drift $\mathbf{v_M} \cdot \nabla\alpha$ for the transport analysis of experimental discharges

- Compare correct calculation against DKES-like calculation with $\mathbf{v_M} \cdot \nabla\alpha = 0$ ($\mathbf{v}_E \cdot \nabla\psi \sim \varphi_1$ is set to 0 in both cases).
- Input: **experimental profiles** and configuration (EIM) of W7-X shot #180918041 [Estrada (2021) NF].
  - High performance, reduced turbulent contribution to ion energy transport.
- Well-known qualitative behaviour: peak in Q_i reduced and moved towards negative E_r (opposite effect, not shown, for the electrons).
- **Results change quantitatively**: neoclassical flux is 10 % larger:
  - Relative weight of neoclassical/ turbulent transport not altered.
  - Effect is small but **systematic**.





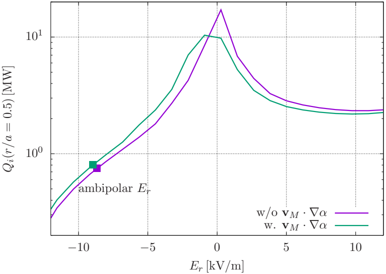
Parameter dependence of the role of the tangential magnetic drift $\mathbf{v_M} \cdot \nabla\alpha$

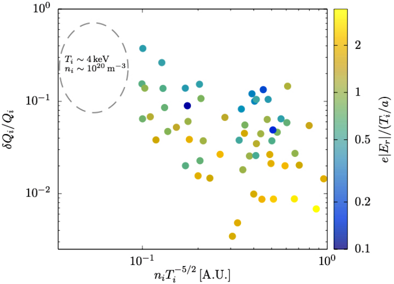
Effect of tangential magnetic drift, not so large in W7-X due to large aspect ratio.

- Large in LHD [Velasco, JCP (2020)].
- Larger for the high-mirror (KJM) configuration of W7-X, specially at higher β due to diamagnetic effect.
- Even for standard (EIM) configuration of W7-X, will become important at higher temperature.

Repeat comparison using representative profiles from [Carralero, EPS (2021)]:

- $\delta Q_i/Q_i$ large for small $n_i T_i^{-5/2}$ and $|E_r|$.
- $\delta Q_i/Q_i \sim 1$ possible in next campaigns of W7-X.





Summary

We have shown that KNOSOS is a **powerful low-collisionality neoclassical code** that:

- is extremely fast, and at the same time,
- can calculate physical effects usually neglected: tangential magnetic drift and φ_1.

There is a wide variety of plasma physics problems that it can be applied to:

- analysis of experimental discharges,
- stellarator optimization (installed at CIEMAT branch of STELLOPT; part of EUROfusion's main (TSVV) task on stellarator optimization),
- input for impurity transport simulations (E_r and φ_1) and for gyrokinetic simulations (distribution function g_b) and other transport simulations (D_{11} to e.g. neotransp).

KNOSOS **is publicly available** at

https://github.com/joseluisvelasco/KNOSOS