Orbit-averaged approach to fast-ion transport in stellarators

Iván Calvo[1], José Luis Velasco[1] and Félix I. Parra[2]

[1] *Laboratorio Nacional de Fusión, CIEMAT, Madrid, Spain*

[2] *Princeton Plasma Physics Laboratory, Princeton, USA*

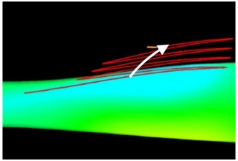
European Fusion Theory Conference

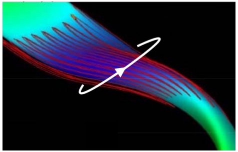
Padova, Italy, 4 October 2023

Motivation

- In a reactor, alpha particles must be well confined so that they have time to transfer their energy to the bulk plasma and damage to plasma-facing components is avoided.

- In a non-optimized stellarator, trapped orbits are not confined.
  - Large neoclassical transport of thermal particles at low collisionality.
- Worse for alpha particles because they do not not enjoy the confining effect of the $\mathbf{E} \times \mathbf{B}$ drift tangent to flux surfaces.
  - **Good fast-ion confinement is a demanding criterion in stellarator optimization.**

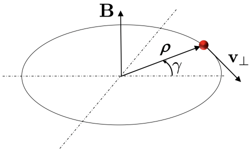




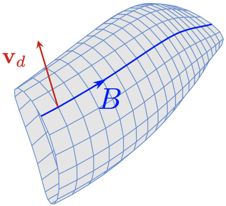
The understanding of fast-ion transport and the development of efficient numerical tools are important for current experiments and for the design of stellarator reactors.

Motivation

- Usual tools: Monte Carlo codes that solve either a full-orbit kinetic equation or a drift-kinetic equation (DKE) for guiding centers.
  - ASCOT [Hirvijoki, CPC 2014], ANTS [Drevlak, NF 2014], BEAMS3D [McMillan, PPCF 2014], GNET [Masaoka, NF 2013], SIMPLE [Albert, JPP 2020]...



- Guiding centers move rapidly along **B** and drift across the magnetic field. For some applications, only the dynamics averaged over the rapid motion along **B** (i.e. over lowest-order orbits) should matter.



This talk

- **Derivation of an orbit-averaged DKE for stellarators*.**
  - Reduced phase-space dimensionality w.r.t. guiding-center equations.
  - Gives physical insight into fast-ion transport.
- Implementation in a new Monte Carlo code, `KNOSOS-MC`.

*Related work for tokamaks in [Eriksson, PoP 1994], [Meng, Lauber, this conference] and for model stellarator magnetic fields in [Kolesnichenko, PoP 2006].

Orderings and assumptions

Plasma consisting of bulk ions with mass m_i and charge $Z_i e$, electrons with mass m_e, and fast ions with mass m_h, charge $Z_h e$ and characteristic speed v_h.

- $Z_i \sim Z_h \sim 1$, $m_i \sim m_h$, $v_{ti} \ll v_h \ll v_{te}$.
- Strongly magnetized fast ions: $\rho_{h*} = \rho_h / L_0 \ll 1$, where ρ_h is the fast-ion gyroradius and $L_0 \sim R \sim a$ is a characteristic length of the order of the device size.
- Small fast-ion density n_h: the electrostatic potential φ is determined by bulk species and fast-ion self-collisions are negligible.
- $\varphi \simeq \varphi_0$, where φ_0 is a flux function.
- $\rho_{h*} \sim \nu_{h*}$, where ν_{h*} is the fast-ion collisionality.

Typical values of NBI hydrogen ions in W7-X and alpha particles in a Helias reactor HSR4/18.

	R	a	B	T_i	T_e	$\frac{1}{2}m_h v_h^2$	v_{ti}/v_h	v_h/v_{te}	ρ_h/a
W7-X	5.5	0.5	2.6	1.5	3	60	0.158	0.104	0.027
HSR4/18	18	2	5	15	15	3500	0.083	0.178	0.024

Full-orbit kinetic equation

- Under the above assumptions, the equation for the fast-ion distribution $f_h(\mathbf{x}, \mathbf{v}, t)$ is

$$\partial_t f_h + \mathbf{v} \cdot \nabla f_h + \frac{Z_h e}{m_h}(\mathbf{v} \times \mathbf{B} + \varphi_0) \cdot \nabla_{\mathbf{v}} f_h = C_h[f_h] + S_h,$$

  where S_h is a source and the collision term reads [Helander, CUP 2002]

$$C_h[f_h] = \frac{1}{2\tau_s} v_b^3 \nabla_v \cdot \left(\nabla_v \nabla_v v \cdot \nabla_v f_h \right) + \frac{1}{\tau_s} v_c^3 \nabla_v \cdot \left(\frac{\mathbf{v}}{v^3} f_h \right) + \frac{1}{\tau_s} \nabla_v \cdot (\mathbf{v} f_h) \, .$$

- Here, τ_s is the slowing-down time, and v_c and v_b are the velocities below which the drag and the pitch-angle scattering of the bulk ions start to matter.
- The $\mathbf{E} \times \mathbf{B}$ drift is negligible in our ordering and certainly for alpha particles, but we keep it to be able to check its influence in current experiments.

Drift-kinetic equation

- Expanding the full-orbit kinetic equation in $\rho_{h*} \ll 1$, one can average out the motion of the fast ions around lines of $\mathbf{B}$. The result is the DKE for the guiding centers [Hazeltine, PoF 1973], [d'Herbemont, JPP 2022].
- Velocity coordinates $\{\mathcal{E}, \mu, \sigma, \phi\}$, where $\mathcal{E} = v^2/2 + Z_h e \varphi_0 / m_h$, $\mu = v_\perp^2/2B$, $\sigma = v_{||}/|v_{||}|$ and ϕ is the gyrophase. Here,

$$v_{||}(\mathbf{x}, \mathcal{E}, \mu, \sigma) = \sigma \sqrt{2\left(\mathcal{E} - U(\mathbf{x}, \mu)\right)}, \quad v(\mathbf{x}, \mathcal{E}) = \sqrt{2\left(\mathcal{E} - \frac{Z_h e \varphi_0(\mathbf{x})}{m_h}\right)},$$

$$U(\mathbf{x}, \mu) := \mu B(\mathbf{x}) + \frac{Z_h e \varphi_0(\mathbf{x})}{m_h}.$$

Drift-kinetic equation

- One can show that $f_h \simeq F_h$, where $F_h(\mathbf{x}, \mathcal{E}, \mu, \sigma, t) = (2\pi)^{-1} \int_0^{2\pi} f_h(\mathbf{x}, \mathcal{E}, \mu, \phi, t) \mathrm{d}\phi$.
- The equation for F_h is

$$\partial_t F_h + \dot{\mathbf{x}} \cdot \nabla F_h = C_h[F_h] + \langle S_h \rangle_{\mathrm{gy}}.$$

- Here, $\langle S_h \rangle_{\mathrm{gy}} = \frac{1}{2\pi} \int_0^{2\pi} S_h \mathrm{d}\phi$, and we assume $\langle S_h \rangle_{\mathrm{gy}} \sim \rho_{h*} n_h / L_0 v_h^2$ and $\partial_t \sim \rho_{h*} v_h / L_0$.
- The collision term gives

$$C_h[F_h] = \nu_{hi}^D \frac{v_{||}}{B} \partial_\mu \left(\mu v_{||} \partial_\mu F_h \right) + \frac{v_{||}}{\tau_s} \left[\partial_{\mathcal{E}} \left(\frac{v^2}{v_{||}} \left(1 + \frac{v_c^3}{v^3} \right) F_h \right) + 2 \left(1 + \frac{v_c^3}{v^3} \right) \partial_\mu \left(\frac{\mu}{v_{||}} F_h \right) \right].$$

- As for the guiding-center* trajectories, $\dot{\mathbf{x}} = v_{||} \hat{\mathbf{b}} + \mathbf{v}_d$, where $\mathbf{v}_d = \mathbf{v}_M + \mathbf{v}_E$ and

$$\mathbf{v}_M = \frac{1}{\Omega_h} \hat{\mathbf{b}} \times (v_{||}^2 \hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} + \mu \nabla B), \quad \mathbf{v}_E = \frac{1}{B} \hat{\mathbf{b}} \times \nabla \varphi_0.$$

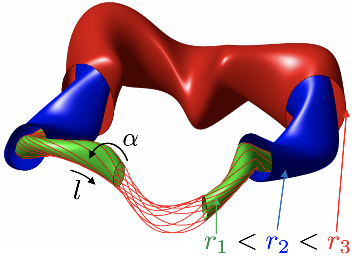
- $|\mathbf{v}_d| / |v_{||}| \sim \rho_{h*} \ll 1$.

*In what follows, we often refer to guiding-center trajectories as particle trajectories.

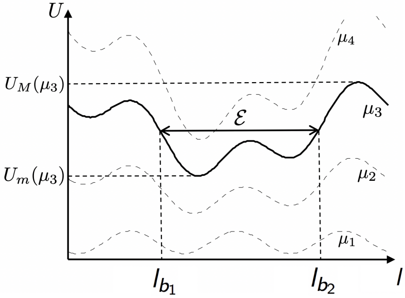
Orbit-averaged DKE: coordinates and lowest-order orbits

- Coordinates $\{r, \alpha, l\}$ adapted to the magnetic field.
- Expand the DKE in $\rho_{h*} \ll 1$ for $\nu_{h*} \sim \rho_{h*}$.
- $F_h = F_h^{(0)} + F_h^{(1)} + \ldots$ **To lowest order, orbits follow magnetic field lines** and

$$v_{||}\hat{\mathbf{b}} \cdot \nabla F_h^{(0)} = 0.$$



- $U := \mu B + Z_h e\varphi_0/m_h$ and let $U_M(\mu)$ be the maximum of U on the flux surface for fixed μ. If $\mathcal{E} < U_M(\mu)$, trapped. If $\mathcal{E} > U_M(\mu)$, passing.
- For trapped particles, $F_h^{(0)} \equiv F_h^{(0)}(r, \alpha, \mathcal{E}, \mu, t)$. For passing particles, $F_h^{(0)} \equiv F_h^{(0)}(r, \mathcal{E}, \mu, \sigma, t)$.
- $F_h^{(0)}$ obtained averaging next-order terms of the DKE.



Orbit-averaged DKE for trapped fast ions

- The equation that determines $F_h^{(0)}(r, \alpha, \mathcal{E}, \mu, t)$ for trapped particles is

$$\partial_t F_h^{(0)} + \overline{\mathbf{v}_d \cdot \nabla r}\, \partial_r F_h^{(0)} + \overline{\mathbf{v}_d \cdot \nabla \alpha}\, \partial_\alpha F_h^{(0)} = \overline{C_h[F_h^{(0)}]} + \overline{S_h}\,,$$

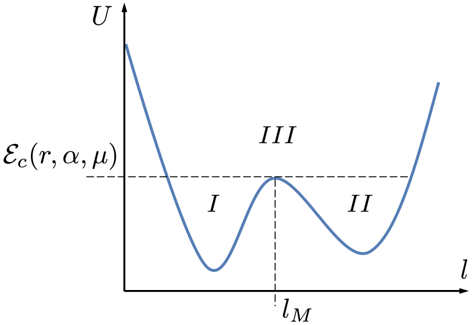
  where $\overline{(\cdot)} = \tau_b^{-1} \sum_\sigma \int_{l_{b_1}}^{l_{b_2}} |v_{||}|^{-1}(\cdot)\mathrm{d}l$ and $\tau_b = 2\int_{l_{b_1}}^{l_{b_2}} |v_{||}|^{-1}\mathrm{d}l$ is the orbit time.
- $J(r, \alpha, \mathcal{E}, \mu) = 2\int_{l_{b_1}}^{l_{b_2}} |v_{||}|\mathrm{d}l$, called *second adiabatic invariant*, is the invariant corresponding to the average over lowest-order orbits of trapped particles.
- Relation between the average of $\mathbf{v}_d$ and J:

$$\overline{\mathbf{v}_d \cdot \nabla r} = \frac{m_h}{Z_h e \Psi_t' \tau_b}\partial_\alpha J, \quad \overline{\mathbf{v}_d \cdot \nabla \alpha} = -\frac{m_h}{Z_h e \Psi_t' \tau_b}\partial_r J,$$

  where Ψ_t' is the derivative with respect to r of the toroidal flux.
- In the absence of collisions, **trapped particles move along curves of constant** J.

Orbit-averaged DKE for trapped fast ions: junctures connecting wells

- **The invariance of J can break at junctures**, where particles undergo transitions between different types of wells.
- These collisionless transitions, where the value of J changes abruptly, are the cause of fast-ion stochastic transport [Beidler, PoP 2001], [Kolesnichenko, PoP 2022].
- **For exactly zero collision frequency, $F_h^{(0)}$ can be discontinuous at junctures.**



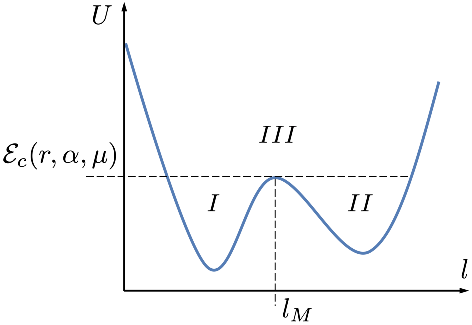
- Apply techniques from [d'Herbemont, JPP 2022] to derive the discontinuity condition by imposing conservation of the collisionless particle flux:

$$F_{h,I}^{(0)} \left(\partial_\alpha J_I \partial_r \mathcal{E}_c - \partial_r J_I \partial_\alpha \mathcal{E}_c\right) + F_{h,II}^{(0)} \left(\partial_\alpha J_{II} \partial_r \mathcal{E}_c - \partial_r J_{II} \partial_\alpha \mathcal{E}_c\right) =$$

$$F_{h,III}^{(0)} \left(\partial_\alpha J_{III} \partial_r \mathcal{E}_c - \partial_r J_{III} \partial_\alpha \mathcal{E}_c\right).$$

Orbit-averaged DKE for trapped fast ions: junctures connecting wells

- **For finite collision frequency, $F_h^{(0)}$ is continuous, but $\partial_\mu F_h^{(0)}$ is not.**
- The relation between the values of $\partial_\mu F_h^{(0)}$ on each side of the juncture is obtained from conservation of the collisional particle flux:



$$\tau_{b,I} \left(\overline{B^{-1} v_{||}^2} \right)_I \partial_\mu F_{h,I} + \tau_{b,II} \left(\overline{B^{-1} v_{||}^2} \right)_{II} \partial_\mu F_{h,II} = \tau_{b,III} \left(\overline{B^{-1} v_{||}^2} \right)_{III} \partial_\mu F_{h,III}.$$

Orbit-averaged DKE for passing fast ions

- The equation that determines $F_h^{(0)}(r, \mathcal{E}, \mu, \sigma, t)$ for passing fast ions is

$$\partial_t F_h^{(0)} = \left\langle \frac{B}{v_{||}} \right\rangle_r^{-1} \left\langle \frac{B}{v_{||}} C_h[F_h^{(0)}] \right\rangle_r + \left\langle \frac{B}{v_{||}} \right\rangle_r^{-1} \left\langle \frac{B}{v_{||}} S_h \right\rangle_r .$$

  Here, $\langle \cdot \rangle_r$ denotes flux-surface average and we have used that, for passing particles, $\partial_\alpha F_h^{(0)} \equiv 0$ and $\langle \mathbf{v}_d \cdot \nabla r \rangle_r \equiv 0$.

Implementation in a Monte Carlo code

Preparatory manipulations

- Redefine the distribution function so that it absorbs the phase-space volume element:

$$G_t(r,\alpha,\mathcal{E},\mu,t) = 2\pi\Psi'_t\tau_b F_h^{(0)} \text{ (trapped)},\ G_p(r,\mathcal{E},\mu,\sigma,t) = 2\pi V' \left\langle \frac{B}{v_{||}} \right\rangle_r F_h^{(0)} \text{ (passing)}.$$

- **Equation for trapped particles**

$$\partial_t G_t = -\partial_r\left(\overline{\mathbf{v}_d\cdot\nabla r}\, G_t\right) - \partial_\alpha\left(\overline{\mathbf{v}_d\cdot\nabla\alpha}\, G_t\right) - \partial_{\mathcal{E}}\left(V^{\mathcal{E}} G_t\right) - \partial_\mu\left(V_t^\mu G_t\right) + \partial_\mu^2\left(D_t G_t\right) + 2\pi\Psi'_t\tau_b\overline{S_h}\,,$$

$$V^{\mathcal{E}} := -\frac{v^2}{\tau_s}\left(1+\frac{v_c^3}{v^3}\right),\ V_t^\mu := -\left[\nu_{hi}^D\left(\mu - \overline{B^{-1}v_{||}^2}\right) + \frac{2}{\tau_s}\left(1+\frac{v_c^3}{v^3}\right)\mu\right],\ D_t := \nu_{hi}^D\,\mu\,\overline{B^{-1}v_{||}^2}\,.$$

- **Equation for passing particles**

$$\partial_t G_p = -\partial_{\mathcal{E}}\left(V^{\mathcal{E}} G_p\right) - \partial_\mu\left(V_p^\mu G_p\right) + \partial_\mu^2\left(D_p G_p\right) + 2\pi V'\left\langle \frac{B}{v_{||}} S_h\right\rangle_r,$$

$$V_p^\mu := -\left[\nu_{hi}^D\left(\mu - \left\langle B/v_{||}\right\rangle_r^{-1}\left\langle v_{||}\right\rangle_r\right) + \frac{2}{\tau_s}\left(1+\frac{v_c^3}{v^3}\right)\mu\right],\ D_p := \nu_{hi}^D\mu\left\langle B/v_{||}\right\rangle_r^{-1}\left\langle v_{||}\right\rangle_r.$$

Stochastic differential equations

- Once the orbit-averaged DKE is written in terms of G_t and G_p, it is easy to infer the equivalent stochastic differential equations by resorting to standard results in the mathematical literature.
- Let $r(t)$, $\alpha(t)$, $\mathcal{E}(t)$, $\mu(t)$ and $\sigma(t)$ be random variables.

- **Itô stochastic differential equations for trapped particles**

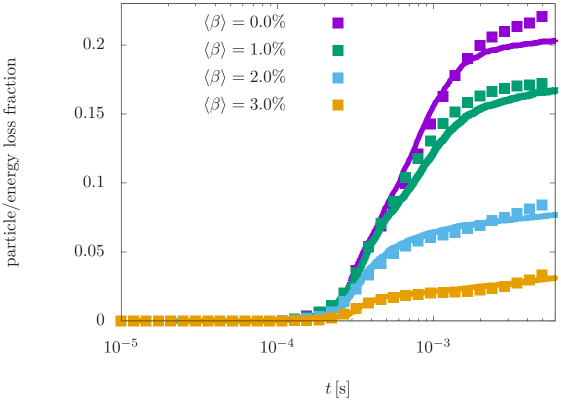
$$\mathrm{d}r = \overline{\mathbf{v}_d \cdot \nabla r}\,\mathrm{d}t, \quad \mathrm{d}\alpha = \overline{\mathbf{v}_d \cdot \nabla \alpha}\,\mathrm{d}t, \quad \mathrm{d}\mathcal{E} = V^{\mathcal{E}}\,\mathrm{d}t, \quad \mathrm{d}\mu = V_t^{\mu}\,\mathrm{d}t + \sqrt{2D_t}\,\mathrm{d}W,$$

where $\mathrm{d}W(t)$ is a Wiener process.

- **Itô stochastic differential equations for passing particles**

$$\mathrm{d}r = 0, \quad \mathrm{d}\mathcal{E} = V^{\mathcal{E}}\mathrm{d}t, \quad \mathrm{d}\mu = V_p^{\mu}\mathrm{d}t + \sqrt{2D_p}\,\mathrm{d}W, \quad \mathrm{d}\sigma = 0.$$

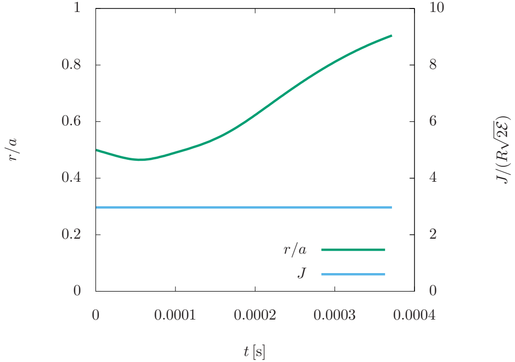
KNOSOS-MC: collisionless simulations

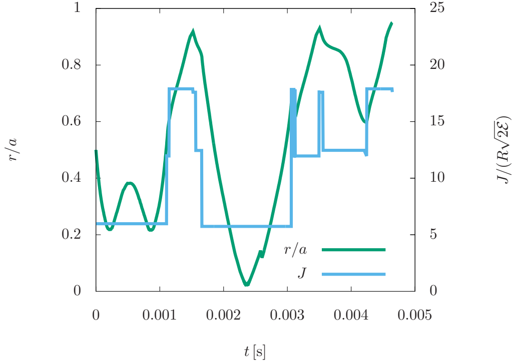


- Collisionless simulations of alpha losses in a W7-X configuration scaled to reactor size.
- Alpha particles are born at $r/a = 0.5$.
- Agreement between `KNOSOS-MC` (squares) and guiding-center simulations with `ASCOT` (solid curves).
  - Estimation of orbit width added to `KNOSOS-MC` for meaningful comparison.
- Phases dominated by prompt losses and by stochastic losses clearly distinguished.

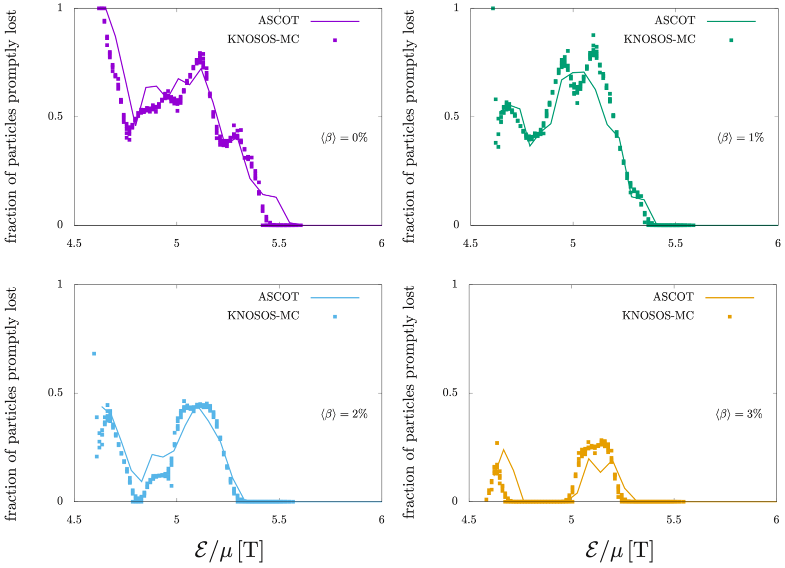
KNOSOS-MC: collisionless simulations

- J as a function of time for a particle that is promptly lost and for a particle that is lost by stochastic mechanisms.



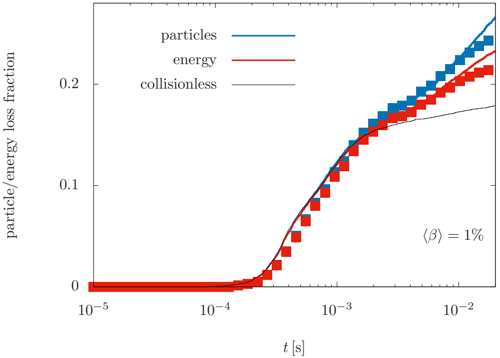


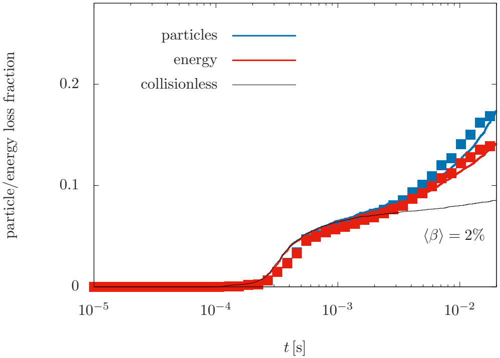
KNOSOS-MC: collisionless simulations



- Prompt losses vs $\mathcal{E}/\mu$ for the above simulations.
- Important information to guide the optimization of magnetic configurations.

KNOSOS-MC: simulations including collisions





- Simulations of alpha particle and energy losses including collisions.
- Agreement between KNOSOS-MC (squares) and guiding-center simulations with ASCOT (solid curves).

Conclusions and further work

- Orbit-averaged drift-kinetic equation for fast-ion transport in general stellarator geometry derived.
  - Radially global, includes collisions, and accounts for both trapped and passing particles.
  - Careful treatment of junctures between different types of wells.
- Equation implemented in a new Monte Carlo code, `KNOSOS-MC`. Examples support the validity of the orbit-averaged approach.

Next steps

- Exploitation of `KNOSOS-MC`.
- Finite-difference code that calculates the steady state of the new equation.
  - Reduction of dimensionality by 1 w.r.t. `KNOSOS-MC` and by 2 w.r.t. guiding-center codes.

Paper in preparation

Orbit-averaged drift-kinetic equation for fast-ion transport in stellarators, I. Calvo, J. L. Velasco and F. I. Parra.