Fast modelling of energetic ion neoclassical losses in stellarators

José Luis Velasco[1],
I. Calvo[1], S. Mulas[1], E. Sánchez[1], F.I. Parra[2], A. Cappa[1]

[1]Laboratorio Nacional de Fusión, CIEMAT
2 Rudolf Peierls Centre for Theoretical Physics, University of Oxford

Wistell meeting April 23, 2021

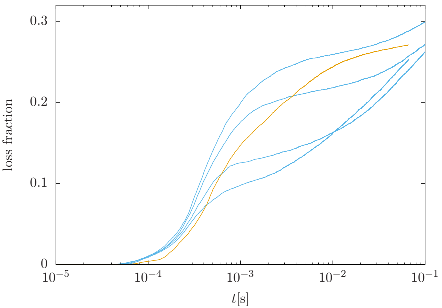
Goal

Energetic ions are lost via neoclassical mechanisms in stellarators. Two basic time scales:

- Prompt losses.
- Stochastic losses.

Prompt losses correspond to energetic ions of higher kinetic energy:

- Deleterious effect.
- Modelling can be collisionless, limited to trapped ions and without E_r.



(In all this work: collisionless simulations with ASCOT, 50 keV ions mimicking α distribution).

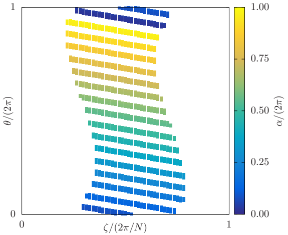
Goal of this work: develop a **fast <u>model</u> for the evaluation of prompt losses of energetic ions in stellarators** (paper to be submitted).

- Useful for optimization and characterization of parameter space, but also for understanding key features.

Long term goal: **fast and <u>accurate</u> simulations of energetic ions** (in preparation, final slides).

Notation

- Spatial coordinates: normalized toroidal flux ($s = \Psi_t/\Psi_{LCMS}$), field label ($\alpha = \theta - \iota\zeta$) and arc length ($l$).
- Velocity coordinates: velocity (v) and pitch angle ($\lambda = 2\mu/v^2$). Constants of motion.



For trapped particles:

$$\overline{\mathbf{v}_M \cdot \nabla s} = \frac{m}{Ze\Psi_t\tau_b}\partial_\alpha J\,, \qquad \overline{\mathbf{v}_M \cdot \nabla \alpha} = -\frac{m}{Ze\Psi_t\tau_b}\partial_s J$$

$$J(s,\alpha,v,\lambda) = 2v\int_{l_{b_1}}^{l_{b_2}} \mathrm{d}l\sqrt{1-\lambda B}\,, \quad \overline{f} = \frac{2}{v\tau_b}\int_{l_{b_1}}^{l_{b_2}} \mathrm{d}l\frac{f}{\sqrt{1-\lambda B}}\,, \quad \tau_b = \frac{2}{v}\int_{l_{b_1}}^{l_{b_2}} \frac{\mathrm{d}l}{\sqrt{1-\lambda B}}$$

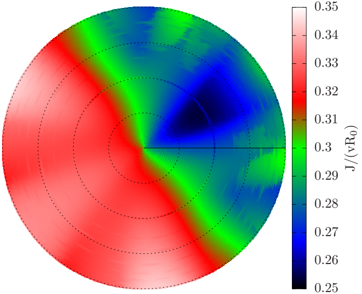
($f(s,\alpha,l,\lambda,v)$ is an arbitrary function).

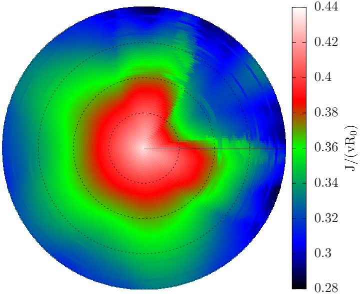
- $|\partial_\alpha J/\partial_s J|$ small: poloidal precession on the flux-surface.
- $|\partial_\alpha J/\partial_s J|$ large: large radial excursions, **superbanana orbits**.

Energetic ions move in (s,α) space at constant J.

Energetic ion confinement and contours of J

$\beta = 1\,\%$ $(\lambda = 0.41/\mathrm{T})$ $\beta = 4\,\%$





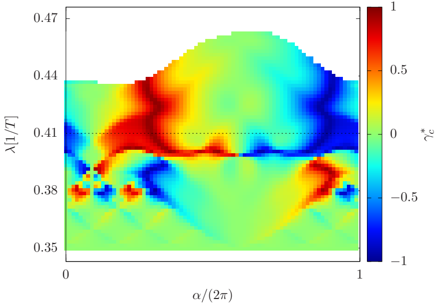
- For W7-X (KJM configuration), when β increases, $J-$ contours tend to be aligned to $s-$contours and J tends to be monotonically decreasing with s: maximum-J property [Helander, PoP (2013)].
- Configurations satisfying exactly the maximum$-J$ condition have no superbananas, because $\partial_s J$ does not vanish.

Radially local description of J-maps: why?

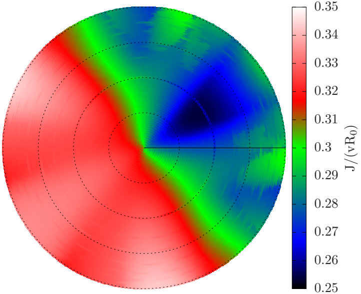
- Radially global description requires a radially global code:
  - Does not exist, except for guiding-center MC codes (but see final slides!).
  - Additional radial variable $\Rightarrow$ higher computing cost.
- Stellarator optimization tends to use radially local approach:
  - Targets, proxies... evaluated at discrete flux-surfaces.
  - Theory predicts that perfect optimization (w.r.t some criteria) cannot be achieved in the full volume ([Garren and Boozer, PoF (1991)] in the case of quasisymmetry).
  - Optimizing a single flux-surface can be successful strategy [Henneberg, NF (2019)]
  - Specific of energetic ions: perfectly optimized flux surface $s = s_0$ confines all energetic ions born at $s \leq s_0$.

Radially local description of J-maps: γ_c^*

$\gamma_c^*(\alpha,\lambda)$ at $s=0.25$



$J(s,\alpha)$ polar map for $\lambda = 0.41$ /T

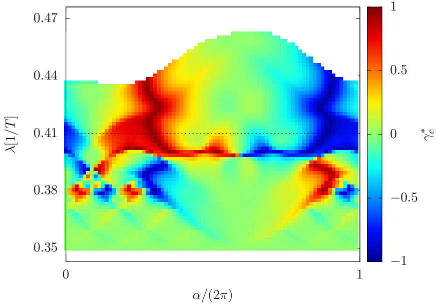


$$\gamma_c^* = \frac{2}{\pi}\,\mathrm{arctan}\,\frac{\partial_\alpha J}{|\partial_s J|} = \frac{2}{\pi}\,\mathrm{arctan}\,\frac{\overline{\mathbf{v}_M\cdot\nabla s}}{|\overline{\mathbf{v}_M\cdot\nabla\alpha}|}$$

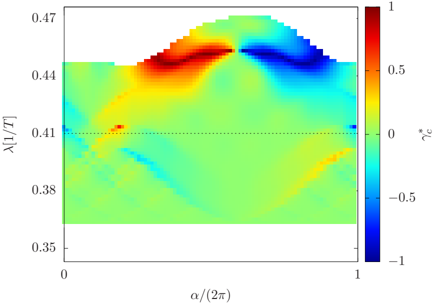
- $\gamma_c^* = 0$ where s-contours and J-contous are well aligned.
- $\gamma_c^* = \pm 1$ where s-contours and J-contous are orthogonal.
  - $\gamma_c^* = +1$ when $\overline{\mathbf{v}_M\cdot\nabla s}$ is directed outwards.

Interpretation of γ_c^* maps

$\beta = 1\,\%, s = 0.25$



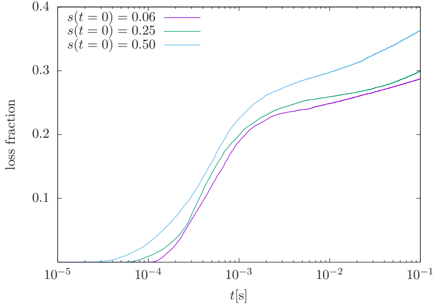
$\beta = 4\,\%, s = 0.25$



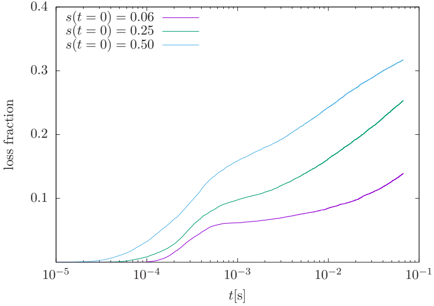
- When β increases, superbananas move to larger values of λ.
- Globally, the weight of the superbananas (area of the red and blue region in γ_c^* map) is reduced.
- ASCOT simulations confirm improvement of energetic ion loss fraction.
  - Can we use these maps to perform predictions?

Qualitative validation of γ_c^* maps with ASCOT calculations

$\beta = 1\,\%$

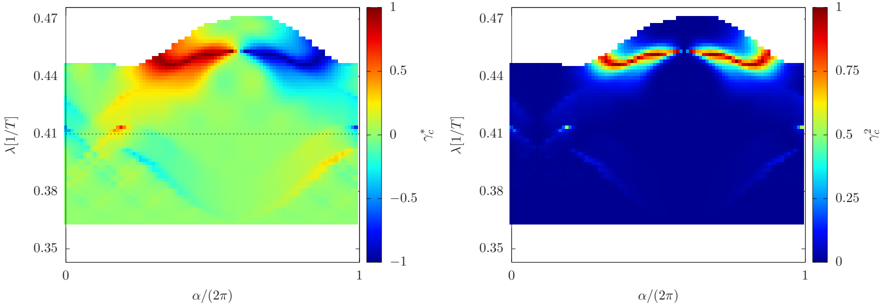


$\beta = 4\,\%$



- When β increases, superbananas move to larger values of λ.
- Globally, the weight of the superbananas (area of the red and blue region in γ_c^* map) is reduced.
- ASCOT simulations confirm improvement of energetic ion loss fraction.
  - Can we use these maps to perform predictions?

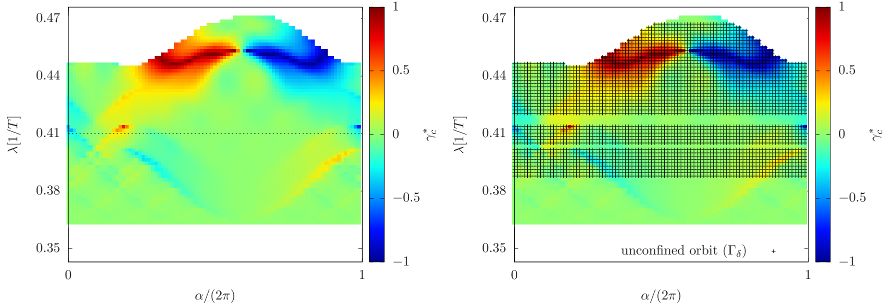
The Γ_c proxy



Proxy Γ_c [Nemov, PoP (2008)] is roughly an integral of $(\gamma_c^*)^2$.

- Measure of separation of J-contours from s-contours.
- Reduction of Γ_c typically correlates with improvement of energetic ion confinement.
- Employed succesfully in optimization of QHS [Bader, JPP (2019)].
  - Can we go beyond this qualitative assesment?

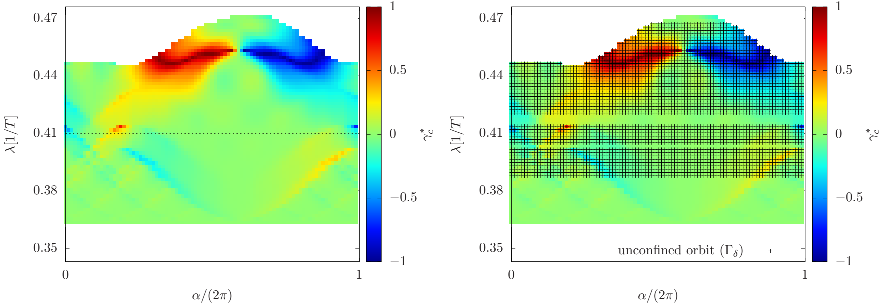
First approximation to modelling the fraction of losses



- Ions move at constant λ.
- λ-extension of red region should be greater concern than α-extension.
- Possible model: all ions born with λ where a superbanana exists are lost.
  - More precisely: orbit is unconfined if $\max(\gamma_c^*(\alpha|\lambda)) > \gamma_{th}$.
  - We choose $\gamma_{\rm th} = 0.2$, corresponding approximately to $\frac{\mathbf{v}_M\cdot\nabla s}{\mathbf{v}_M\cdot\nabla\alpha} \approx \frac{1}{\pi}$

$$\Gamma_\delta = \frac{1}{2}\left\langle \int_{B_{\rm MAX}^{-1}}^{B^{-1}} {\rm d}\lambda \frac{B}{\sqrt{1-\lambda B}} H\Big(\max(\gamma_c^*(\alpha|\lambda)) - \gamma_{th}\Big)\right\rangle$$

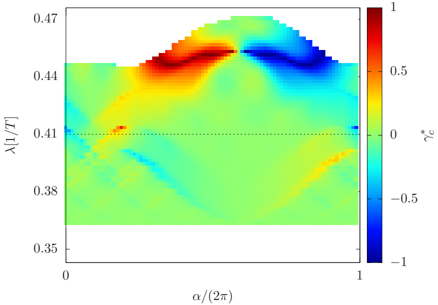
First approximation to modelling the fraction of losses

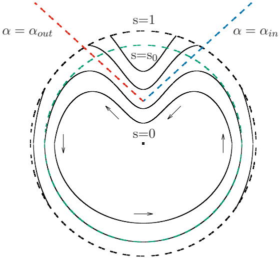


- Ions move at constant λ.
- λ-extension of red region should be greater concern than α-extension.
- Possible model: all ions born with λ where a superbanana exists are lost.
  - More precisely: orbit is unconfined if $\max(\gamma_c^*(\alpha|\lambda)) > \gamma_{th}$.
  - We choose $\gamma_{\rm th} = 0.2$, corresponding approximately to $\frac{\mathbf{v}_M\cdot\nabla s}{\mathbf{v}_M\cdot\nabla\alpha} \approx \frac{1}{\pi}$

$$\Gamma_\delta = \frac{1}{2}\left\langle \int_{B_{\rm MAX}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} H\Big(\max(\gamma_c^*(\alpha|\lambda)) - \gamma_{th}\Big)\right\rangle$$

A (small) step beyond the local approach



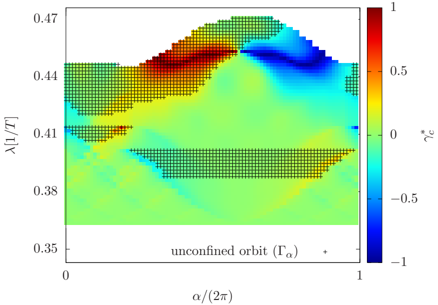


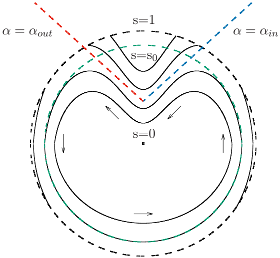
Ions at $s = s_0$ (dashed green) precess in α at constant J (thick black).

- Some ions reach $\alpha \approx \alpha_{out}$, where $\gamma_c^* \approx 1$, and escape.
- Others are tied to s_0 (inwards excursion around α_{in}, where $\gamma_c^* \approx -1$).
- Estimated fraction of prompt losses ($0 < \Gamma_\alpha < f_{\mathrm{trapped}}$):

$$\Gamma_\alpha = \frac{1}{2}\left\langle \int_{B_{\mathrm{MAX}}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} H\left((\alpha_{\mathrm{out}} - \alpha)\, \overline{\mathbf{v}_M \cdot \nabla\alpha}\right) H\left((\alpha - \alpha_{\mathrm{in}})\, \overline{\mathbf{v}_M \cdot \nabla\alpha}\right) \right\rangle$$

A (small) step beyond the local approach



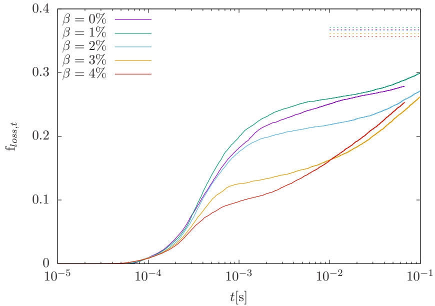


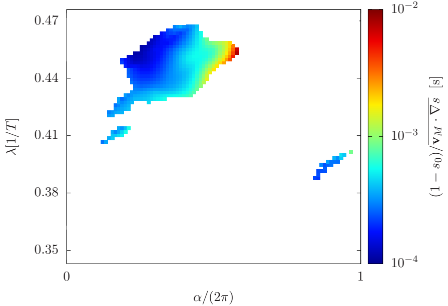
Ions at $s = s_0$ (dashed green) precess in α at constant J (thick black).

- Some ions reach $\alpha \approx \alpha_{out}$, where $\gamma_c^* \approx 1$, and escape.
- Others are tied to s_0 (inwards excursion around α_{in}, where $\gamma_c^* \approx -1$).
- Estimated fraction of prompt losses ($0 < \Gamma_\alpha < f_{\mathrm{trapped}}$):

$$\Gamma_\alpha = \frac{1}{2}\left\langle \int_{B_{\mathrm{MAX}}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} H\Big((\alpha_{\mathrm{out}} - \alpha)\, \overline{\mathbf{v}_M \cdot \nabla\alpha}\Big) H\Big((\alpha - \alpha_{\mathrm{in}})\, \overline{\mathbf{v}_M \cdot \nabla\alpha}\Big)\right\rangle$$

Model validation with ASCOT: time scale and total prompt losses

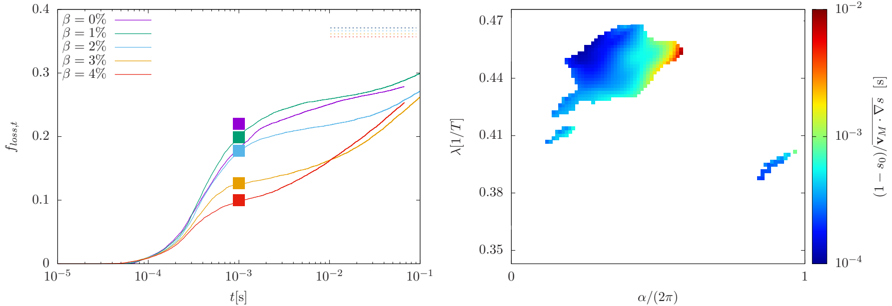




Model (squares) captures well several features of the ASCOT simulations (lines):

- $(1-s_0)/\overline{\mathbf{v}_M \cdot \nabla s}$ evaluated around α_{out} gives the right time scale: 10^{-4} s$< t < 10^{-3}$ s.
- Value of total prompt losses at t *approximately* 10^{-3} s.
- Positive effect of β, even *jump* between 2 % and 3 %.

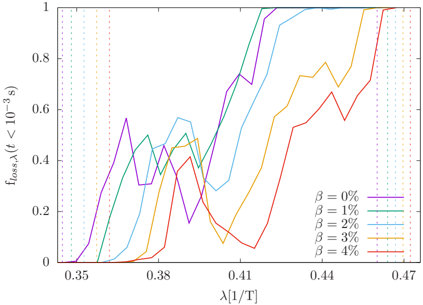
Model validation with ASCOT: time scale and total prompt losses

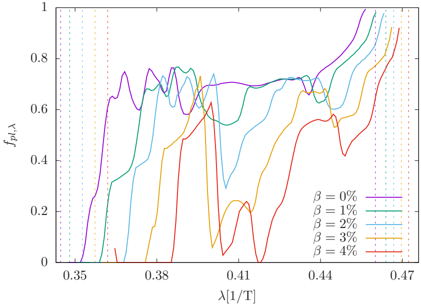


Model (squares) captures well several features of the ASCOT simulations (lines):

- $(1-s_0)/\overline{\mathbf{v}_M \cdot \nabla s}$ evaluated around α_{out} gives the right time scale: 10^{-4} s$< t < 10^{-3}$ s.
- Value of total prompt losses at t *approximately* 10^{-3} s.
- Positive effect of β, even *jump* between 2 % and 3 %.

Model validation with ASCOT: velocity distribution





Model captures well several features:

- For $\beta < 3\,\%$, particles with all velocities are expected to be lost.
- At $\beta = 3\,\%$, some ions with $\lambda \approx 0.41$/T become confined.
- For $\beta > 3\,\%$, a larger range of λ has good confinement.

Model validation: overall configuration performance

Encapsulate performance on a single number (per flux-surface)
$\Rightarrow$ can be employed in a stellarator suite such as STELLOPT.

Two variations w.r.t. Nemov's Γ_c:

$$\check{\Gamma}_\mathrm{c} = \frac{1}{2}\left\langle \int_{B_\mathrm{MAX}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} (\gamma_\mathrm{c}^*)^2 \right\rangle = \frac{\pi}{2\sqrt{2}} \Gamma_\mathrm{c}$$

$$\hat{\Gamma}_\mathrm{c} = \frac{1}{2}\left\langle \int_{B_\mathrm{MAX}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} |\gamma_\mathrm{c}^*| \right\rangle$$

Existence of superbananas:

$$\Gamma_\delta = \frac{1}{2}\left\langle \int_{B_\mathrm{MAX}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} H\Big(\max(\gamma_\mathrm{c}^*(\alpha|\lambda)) - \gamma_{th}\Big) \right\rangle$$

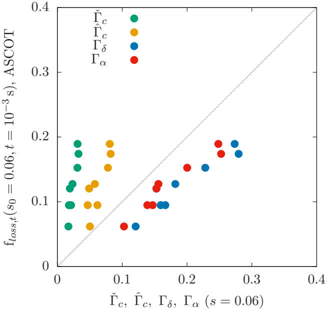
Our final model:

$$\Gamma_\alpha = \frac{1}{2}\left\langle \int_{B_\mathrm{MAX}^{-1}}^{B^{-1}} \mathrm{d}\lambda \frac{B}{\sqrt{1-\lambda B}} H\Big((\alpha_\mathrm{out} - \alpha)\, \overline{\mathbf{v}_M \cdot \nabla\alpha}\Big) H\Big((\alpha - \alpha_\mathrm{in})\, \overline{\mathbf{v}_M \cdot \nabla\alpha}\Big) \right\rangle$$

Model validation: overall configuration performance

- Repeat the calculation for main configurations of the OP1.2 campaign: KJM (incl. β scan), EIM, DBM, FTM.
- Compare:
  - Fraction of prompt losses for ions born at $s = 0.06$ calculated with ASCOT (y axis)
  - Model prediction at $s = 0.06$ (x axis).

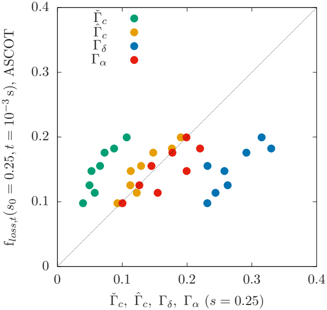
- Γ_α consistently outperforms other proxies (closer to diagonal).
- Γ_α good quantity for stellarator optimization.
- Optimization of just outer surface could be a good idea.



Model validation: overall configuration performance

- Repeat the calculation for main configurations of the OP1.2 campaign: KJM (incl. β scan), EIM, DBM, FTM.
- Compare
  - Fraction of prompt losses for ions born at $s = 0.25$ calculated with ASCOT (y axis)
  - Model prediction at $s = 0.25$ (x axis).

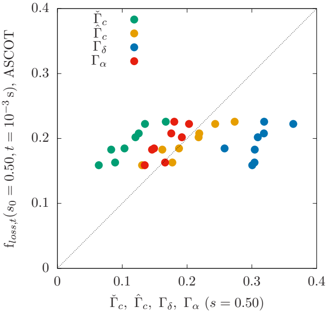
- Γ_α consistently outperforms other proxies (closer to diagonal).
- Γ_α good quantity for stellarator optimization.
- Optimization of just outer surface could be a good idea.



Model validation: overall configuration performance

- Repeat the calculation for main configurations of the OP1.2 campaign: KJM (incl. β scan), EIM, DBM, FTM.
- Compare
  - Fraction of prompt losses for ions born at $s = 0.50$ calculated with ASCOT (y axis)
  - Model prediction at $s = 0.50$ (x axis).

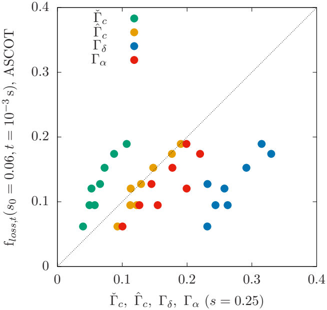
- Γ_α consistently outperforms other proxies (closer to diagonal).
- Γ_α good quantity for stellarator optimization.
- Optimization of just outer surface could be a good idea.



Model validation: overall configuration performance

- Repeat the calculation for main configurations of the OP1.2 campaign: KJM (incl. β scan), EIM, DBM, FTM.
- Compare
  - Fraction of prompt losses for ions born at $s = 0.06$ calculated with ASCOT (y axis)
  - Model prediction at $s = 0.25$ (x axis).

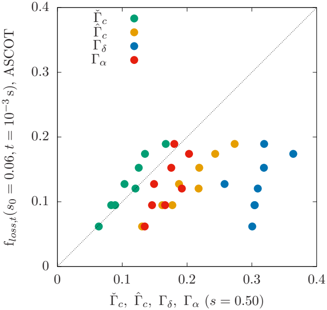
- Γ_α consistently outperforms other proxies (closer to diagonal).
- Γ_α good quantity for stellarator optimization.
- Optimization of just outer surface could be a good idea.



Model validation: overall configuration performance

- Repeat the calculation for main configurations of the OP1.2 campaign: KJM (incl. β scan), EIM, DBM, FTM.
- Compare
  - Fraction of prompt losses for ions born at $s = 0.06$ calculated with ASCOT (y axis)
  - Model prediction at $s = 0.50$ (x axis).

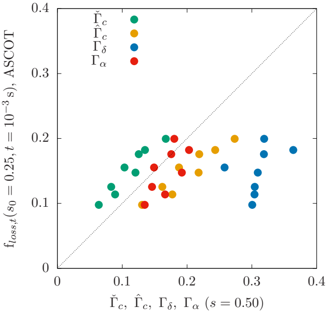
- Γ_α consistently outperforms other proxies (closer to diagonal).
- Γ_α good quantity for stellarator optimization.
- Optimization of just outer surface could be a good idea.



Model validation: overall configuration performance

- Repeat the calculation for main configurations of the OP1.2 campaign: KJM (incl. β scan), EIM, DBM, FTM.
- Compare
  - Fraction of prompt losses for ions born at $s = 0.25$ calculated with ASCOT (y axis)
  - Model prediction at $s = 0.50$ (x axis).

- Γ_α consistently outperforms other proxies (closer to diagonal).
- Γ_α good quantity for stellarator optimization.
- Optimization of just outer surface could be a good idea.

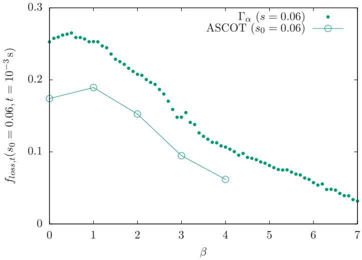


Conclusions

We have developed a model that classifies orbits and succeeds in predicting configuration-dependent aspects of the prompt losses of energetic ions in stellarators.

Calculation takes **a few seconds on a single computer**, useful for:

- Stellarator optimization.
- Parameter scans.



Next steps:

- Should work for other types of stellarators.
- Possible extensions of the model: E_r, pitch-angle collisions, v-diffusion.
- Losses at longer t, associated to stochastic diffusion (but many more subtleties).

But is is clear that **quantitatively correct prediction requires a radially global code.**

- Many features of a particle trajectory are not determined by its initial point in phase space $(s, \alpha, l, \lambda, v)$ but specifically by the initial trapped-orbit in which it lies, $(s, \alpha, \lambda, v) \Rightarrow$ keep on using guiding-center codes but **with a more efficient initial distribution of markers**?

But...

Conclusions and ongoing work

Important theoretical result: bounce-averaged drift-kinetic equations are probably able to describe quantitatively neoclassical fast ion confinement. Need to be radially global.

- If the motion along the field line does not need to be resolved, equation could be solved much faster.
- We are extending (local) code `KNOSOS` to solve rigorously the radially global bounce-averaged drift kinetic equation (i.e., the bounce-averaged version of the equation solved by ASCOT):

$$\partial_t F + \partial_\alpha J \partial_s F - \partial_s J \partial_\alpha F = C(F) + S$$

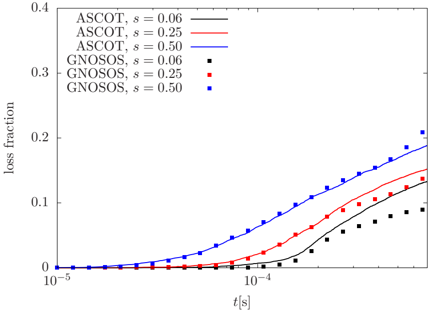
`KNOSOS` $\Rightarrow$ `GNOSOS`: **G**lobal kiNetic Orbit-averaging SOlver for Stellarators

(* provisional name)

This can e.g. be solved by a Monte Carlo method that integrates

$$\begin{aligned} \dot{s} &= \overline{\mathbf{v}_M \cdot \nabla s} = \frac{m}{Ze\Psi_t \tau_b}\partial_\alpha J \\ \dot{\alpha} &= \overline{\mathbf{v}_M \cdot \nabla \alpha} = -\frac{m}{Ze\Psi_t \tau_b}\partial_s J \end{aligned}$$

Conclusions and ongoing work (II)



Working on the longer time scale:

- Stochastic losses have to do with diffusion caused by back and forth transition between trapped states.
  - Transition probabilities need to be calculated accurately.
  - Bounce-averages may need extra accuracy.
- Collision operator different than that of bulk species.