

MONKES: a fast neoclassical code for the evaluation of monoenergetic transport coefficients in stellarator plasmas

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MONKES paper

<https://iopscience.iop.org/article/10.1088/1741-4326/ad3fc9>
<https://github.com/JavierEscoto/MONKES>



MONKES GitHub

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In the past, for general magnetic geometry, **an accurate calculation of the bootstrap current was too slow** to include it in the optimization process.

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In this talk: the code **MONKES** (MONoenergetic Kinetic Equation Solver) will be presented, conceived to satisfy the necessity of fast and accurate calculations of the bootstrap current in stellarators.

Thus, it opens up the possibilities of **direct optimization of neoclassical transport** and to include the bootstrap current effect in **predictive transport simulations**.

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Drift-kinetic equation (DKE)

MONKES solves the same equation as DKES [Hirshman, Phys. Fluids (1986)] for the species a

$$(v\xi\mathbf{b} + \mathbf{v}_E) \cdot \nabla h_a + v \nabla \cdot \mathbf{b} \frac{(1 - \xi^2)}{2} \frac{\partial h_a}{\partial \xi} - \nu^a \mathcal{L} h_a = S_a,$$

where h_a is the deviation of the distribution function from a Maxwellian, $v := |\mathbf{v}|$, $\xi := \mathbf{v} \cdot \mathbf{b}/v$, $\mathbf{v}_E := -E_\psi(\psi) \mathbf{B} \times \nabla \psi / \langle B^2 \rangle$, ψ is the flux-surface label and $\mathcal{L} := \frac{1}{2} \partial/\partial \xi \left((1 - \xi^2) \partial/\partial \xi \right)$.

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The solution to the DKE allows to calculate the neoclassical fluxes

$$\begin{aligned} \langle \Gamma_a \cdot \nabla \psi \rangle &:= \left\langle \int \mathbf{v}_{ma} \cdot \nabla \psi h_a d^3 \mathbf{v} \right\rangle, \\ \langle \mathbf{Q}_a \cdot \nabla \psi \rangle / T_a &:= \left\langle \int v^2 / v_{ta}^2 \mathbf{v}_{ma} \cdot \nabla \psi h_a d^3 \mathbf{v} \right\rangle, \\ \langle n_a \mathbf{V}_a \cdot \mathbf{B} \rangle / B_0 &:= \left\langle B / B_0 \int v \xi h_a d^3 \mathbf{v} \right\rangle. \end{aligned}$$

The source term in the DKE is

$$S_a := f_{Ma} \left[\frac{Bv^2}{\Omega_a} \left(s_1 A_{1a} + (v^2/v_{ta}^2) s_2 A_{2a} \right) + v s_3 A_{3a} \right],$$

where $A_{1a} := n'_a/n_a - 3T'_a/2T_a - e_a E_\psi/T_a$, $A_{2a} := T'_a/T_a$, $A_{3a} := e_a B_0 \langle \mathbf{E} \cdot \mathbf{B} \rangle / T_a \langle B^2 \rangle$ are the thermodynamical forces and

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It is convenient to use a splitting

$$h_a = f_{Ma} \left[\frac{Bv}{\Omega_a} \left(A_{1a} f_1 + A_{2a} (v^2/v_{ta}^2) f_2 \right) + A_{3a} f_3 \right]$$

similar to the one used in [Beidler, NF (2011)].

The splitting is chosen so that $\{f_j\}_{j=1}^3$ are solutions to

$$\xi \mathbf{b} \cdot \nabla f_j + \nabla \cdot \mathbf{b} \frac{(1 - \xi^2)}{2} \frac{\partial f_j}{\partial \xi} - \frac{\widehat{E}_\psi}{\langle B^2 \rangle} \mathbf{B} \times \nabla \psi \cdot \nabla f_j - \hat{\nu} \mathcal{L} f_j = s_j,$$

for $j = 1, 2, 3$, where $\hat{\nu} := \nu(v)/v$ and $\widehat{E}_\psi := E_\psi/v$.

Monoenergetic transport coefficients

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With each solution we can compute the monoenergetic geometric coefficients

$$\widehat{D}_{ij}(\psi, v) := \left\langle \int_{-1}^1 s_i f_j \, d\xi \right\rangle, \quad i, j \in \{1, 2, 3\},$$

which for fixed $(\hat{\nu}, \widehat{E}_\psi)$ depend only on the magnetic geometry.

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At most, four of them are independent: $\{\widehat{D}_{11}, \widehat{D}_{13}, \widehat{D}_{31}, \widehat{D}_{33}\}$. For stellarator-symmetric devices or $E_\psi = 0$ we have the Onsager relation $\widehat{D}_{13} = -\widehat{D}_{31}$.

Using $\hat{D}_{ij}$, the neoclassical fluxes can be calculated using the Onsager matrix

$$\begin{bmatrix} \langle \mathbf{\Gamma}_a \cdot \nabla \psi \rangle \\ \langle \mathbf{Q}_a \cdot \nabla \psi \rangle / T_a \\ \langle n_a \mathbf{V}_a \cdot \mathbf{B} \rangle / B_0 \end{bmatrix} = \begin{bmatrix} L_{11a} & L_{12a} & L_{13a} \\ L_{21a} & L_{22a} & L_{23a} \\ L_{31a} & L_{32a} & L_{33a} \end{bmatrix} \begin{bmatrix} A_{1a} \\ A_{2a} \\ A_{3a} \end{bmatrix}.$$

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The thermal transport coefficients L_{ij} are integrals of the monoenergetic coefficients $\hat{D}_{ij}$

$$L_{ija} := \int_0^\infty 2\pi v^2 f_{Ma} w_i w_j K_{ija} \hat{D}_{ij} dv,$$

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$$\begin{aligned} K_{ija} &:= -\frac{B^2 v^3}{\Omega_a^2}, & i, j \in \{1, 2\}; & \quad K_{3ja} := \frac{B v^2}{\Omega_a}, \quad j \in \{1, 2\}; \\ K_{i3a} &:= -\frac{B v^2}{\Omega_a} = -K_{3ia}, & i \in \{1, 2\}; & \quad K_{33a} := v. \end{aligned}$$

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$$\begin{aligned} L_k &= \frac{k}{2k-1} \left(\mathbf{b} \cdot \nabla + \frac{k-1}{2} \mathbf{b} \cdot \nabla \ln B \right), \\ D_k &= -\frac{\widehat{E}_\psi}{\langle B^2 \rangle} \mathbf{B} \times \nabla \psi \cdot \nabla + \frac{k(k+1)}{2} \hat{\nu}, \\ U_k &= \frac{k+1}{2k+3} \left(\mathbf{b} \cdot \nabla - \frac{k+2}{2} \mathbf{b} \cdot \nabla \ln B \right). \end{aligned}$$

Block Tridiagonal solution: Forward elimination

Starting from $\Delta_{N_\xi} = D_{N_\xi}$ and $\sigma^{(N_\xi)} = s^{(N_\xi)}$ we obtain recursively

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The system is factorized in a lower triangular form

$$L_k f^{(k-1)} + \Delta_k f^{(k)} = \sigma^{(k)}.$$

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- For calculating $\hat{D}_{ij}$ only $\{f^{(k)}\}_{k=0}^2$ are needed. Memory required $\sim O(N_{\text{fs}}^2)$ is minimal and typically fits in a single core.
- The solution requires inverting $N_\xi + 1$ matrices of size N_{fs} . Arithmetical complexity $\sim O(N_{\text{fs}}^3 N_\xi)$ operations. Each inversion can be parallelized.

Block Tridiagonal solution: Backward substitution

Now is immediate to solve the factorized equation for $f^{(k)}$

$$f^{(k)} = \Delta_k^{-1} \left(\sigma^{(k)} - L_k f^{(k-1)} \right), \quad k = 0, 1, \dots, N_\xi.$$

- Discretizing the flux-surface in N_{fs} points, L_k , D_k , U_k and Δ_k are approximated by square matrices of size N_{fs} .
- MONKES employs Boozer angles (θ, ζ) and a pseudospectral Fourier discretization with N_θ and N_ζ points ($N_{\text{fs}} = N_\theta N_\zeta$).
- For calculating $\hat{D}_{ij}$ only $\{f^{(k)}\}_{k=0}^2$ are needed. Memory required $\sim O(N_{\text{fs}}^2)$ is minimal and typically fits in a single core.
- The solution requires inverting $N_\xi + 1$ matrices of size N_{fs} . Arithmetical complexity $\sim O(N_{\text{fs}}^3 N_\xi)$ operations. Each inversion can be parallelized.

This algorithm allows an **accurate** calculation of the $\hat{D}_{ij}$ at (very) low collisionality in ~ 1 minute on a single core. $\Rightarrow$ **MONKES is sufficiently fast for optimization purposes.**

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- ④ **Benchmark and code performance**
- ⑤ Some applications of MONKES
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Study cases for benchmark

Three magnetic configurations are considered. Cases with $\widehat{E}_r = 0$ are in the $1/\nu$ regime and those with $\widehat{E}_r \neq 0$ in the $\sqrt{\nu}$ - ν regime.

Configuration	$\psi/\psi_{\text{lcf}}s$	$\hat{\nu}$ [m^{-1}]	$\widehat{E}_r$ [$\text{kV} \cdot \text{s}/\text{m}^2$]
W7X-EIM	0.200	10^{-5}	0
W7X-EIM	0.200	10^{-5}	$3 \cdot 10^{-4}$
W7X-KJM	0.204	10^{-5}	0
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CIEMAT-QI4	0.250	10^{-5}	0
CIEMAT-QI4	0.250	10^{-5}	10^{-3}

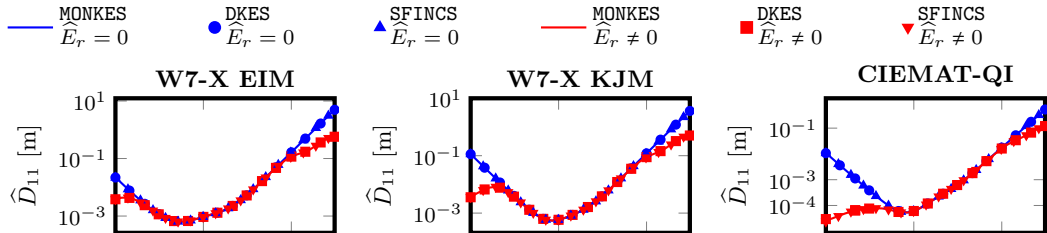
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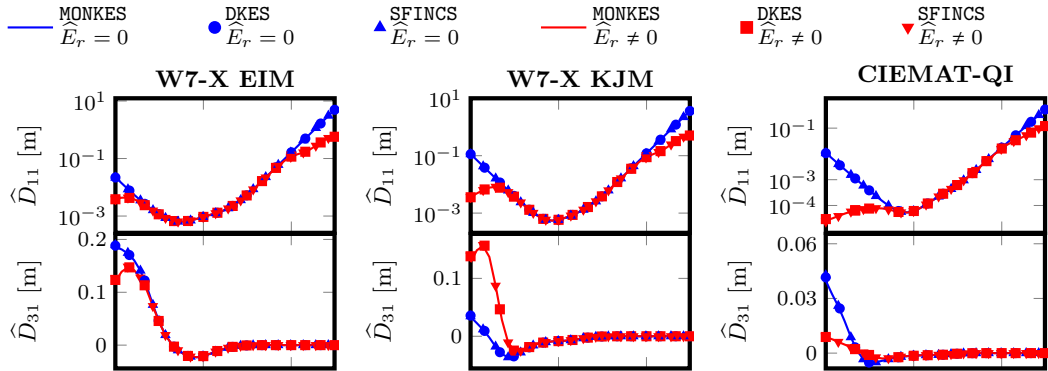
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In order to have a typical value for **MONKES** wall-clock time, we will select resolutions $(N_\theta, N_\zeta, N_\xi)$ for which $\widehat{D}_{31}$ at low collisionality is converged up to 5–7%. This typical value of wall-clock time also gives an upper bound for the wall-clock time required for computing $\widehat{D}_{ij}$ at higher collisionalities.

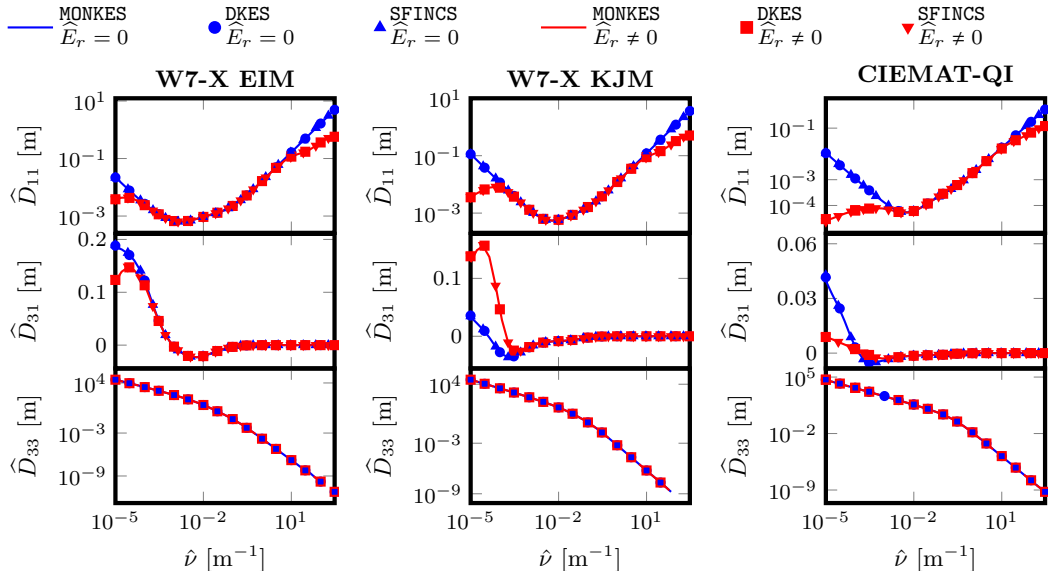
Benchmark of monoenergetic coefficients



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MONKES and DKES wall-clock time for the same level of relative convergence using a single core of CIEMAT's cluster.

Case	$t_{\text{clock}}^{\text{DKES}}$	$t_{\text{clock}}^{\text{MONKES}}$
W7X-EIM $\widehat{E}_r = 0$	90 s	22 s
W7X-EIM $\widehat{E}_r \neq 0$	172 s	35 s
W7X-KJM $\widehat{E}_r = 0$	698 s	31 s
W7X-KJM $\widehat{E}_r \neq 0$	421 s	47 s
CIEMAT-QI4 $\widehat{E}_r = 0$	1060 s	76 s
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MONKES wall-clock time (in seconds) when running in parallel in CIEMAT's cluster.

Case	No. cores			
	2	4	8	16
W7X-EIM $\hat{E}_r = 0$	13	8	5	5
W7X-EIM $\hat{E}_r \neq 0$	20	12	8	6
W7X-KJM $\hat{E}_r = 0$	17	12	7	7
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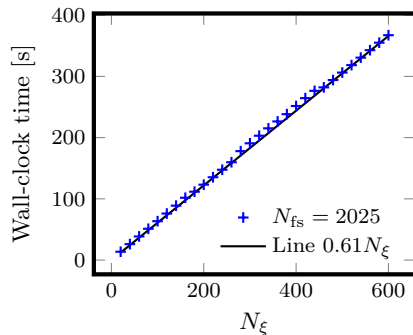
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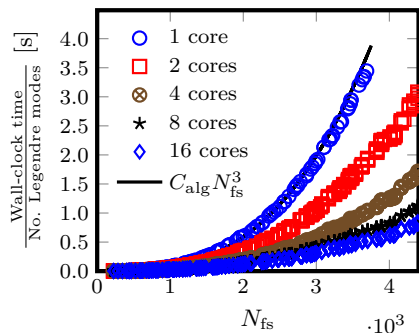
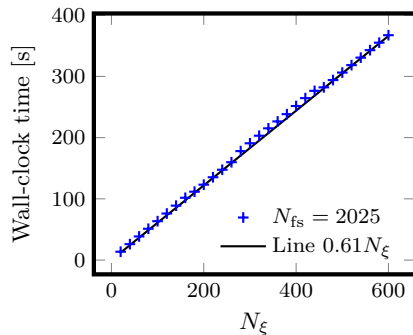
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MONKES is **much faster** than DKES and requires minimal memory resources. MONKES is even faster running in parallel (the CIEMAT-QI cases take 43 s on a laptop with 4 cores).

Arithmetical complexity verification: MONKES wall-clock time $\sim C_{\text{alg}} N_{\xi} N_{\text{fs}}^3$. Wall-clock times for CIEMAT's cluster cores.



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MONKES scales linearly with N_{ξ} and cubically with N_{fs} . For $N_{\text{fs}} \leq 2000$ and $N_{\xi} \leq 200$, rapid calculations (≤ 2 minutes) on a single core.

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Taking advantage of MONKES speed of computation, we can evaluate neoclassically the large database of intermediate configurations $\sim O(10^3)$ obtained during CIEMAT-QI4 optimization campaign, to assess the efficiency of the indirect approach for minimizing $|\hat{D}_{31}|$.

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In order to determine the efficiency of the indirect approach we will investigate whether or not the proxies used for neoclassically optimizing CIEMAT-QI4 correlate with $|\hat{D}_{31}|$ at $\hat{\nu} = 10^{-5} \text{ m}^{-1}$ for $\hat{E}_r = 0$ ($1/\nu$ regime) and $\hat{E}_r \neq 0$ ($\sqrt{\nu}$ - ν regime).

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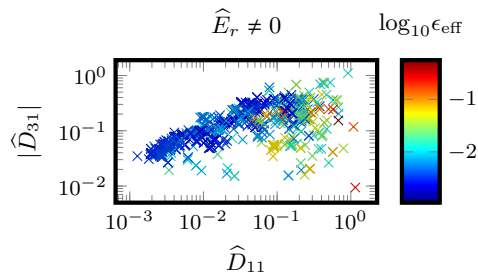
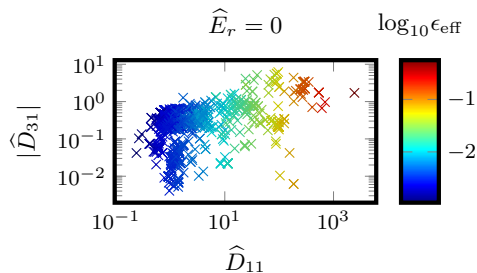
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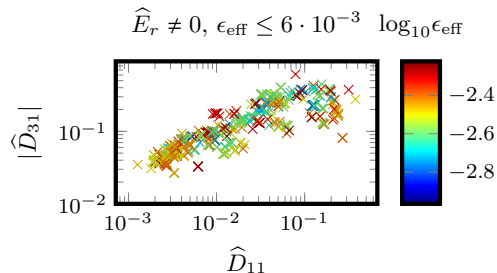
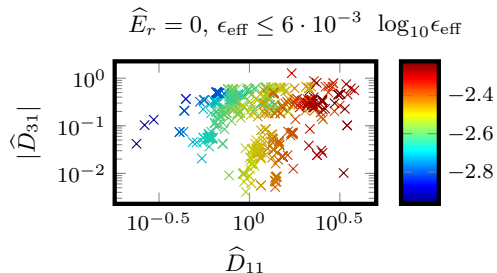
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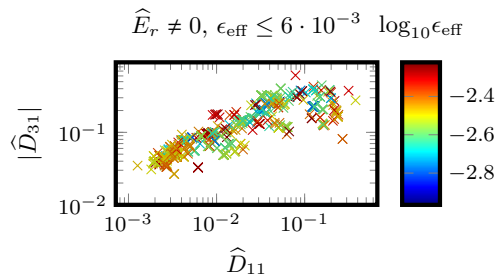
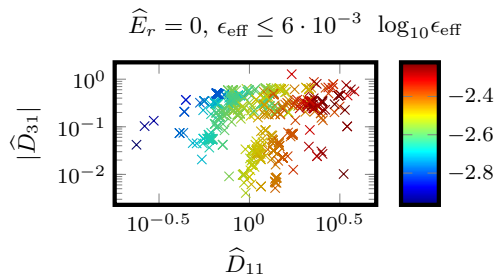
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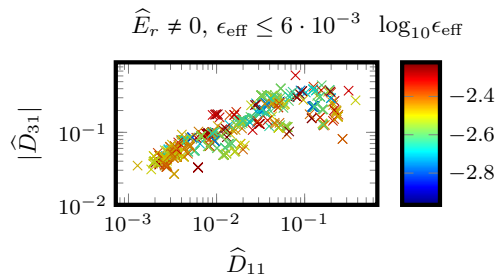
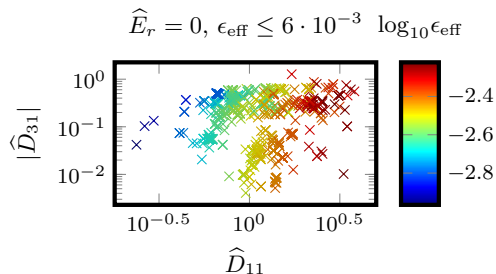
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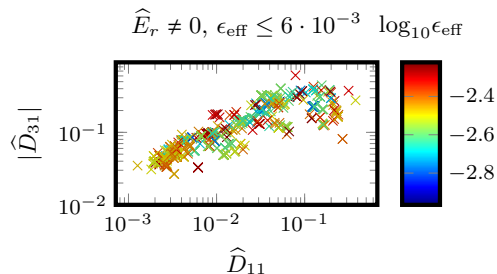
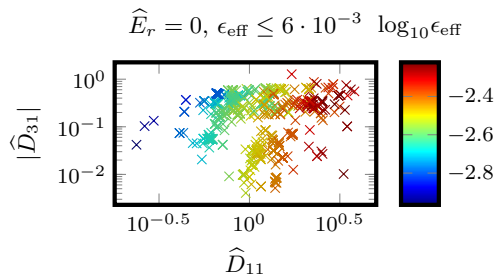
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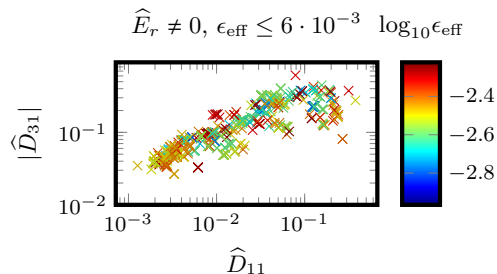
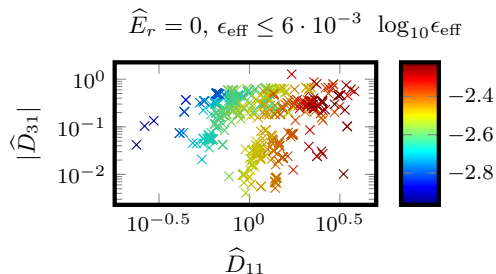
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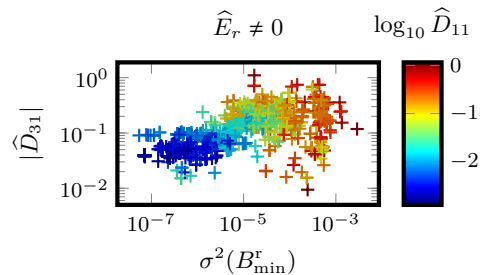
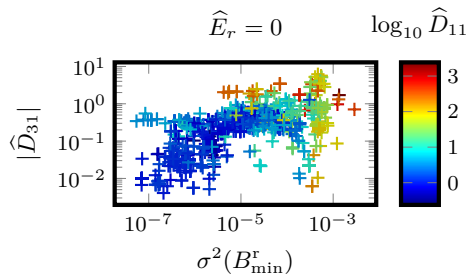
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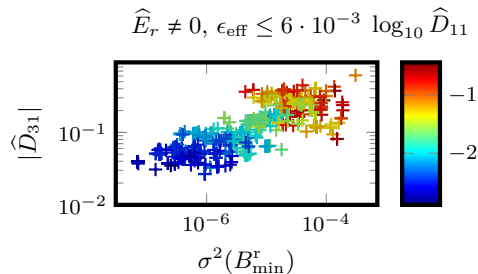
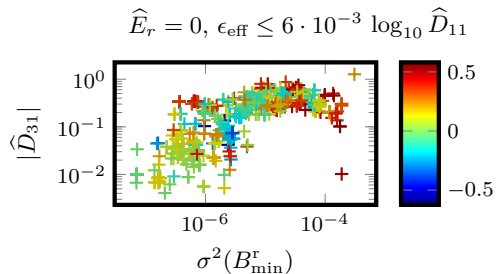


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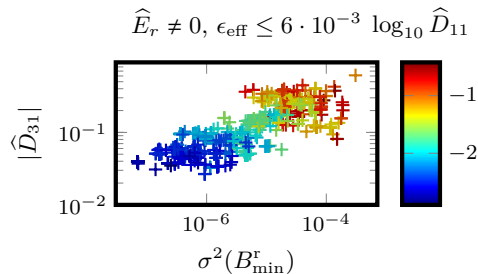
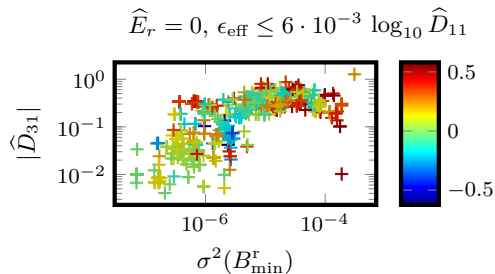
1. Assessment of the efficiency of indirect QI optimization: variance of relative minima



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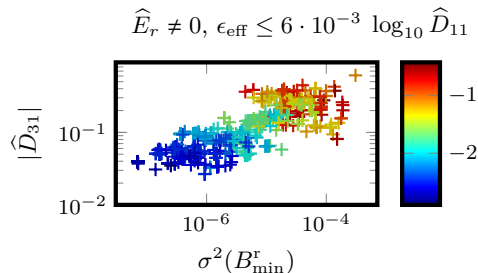
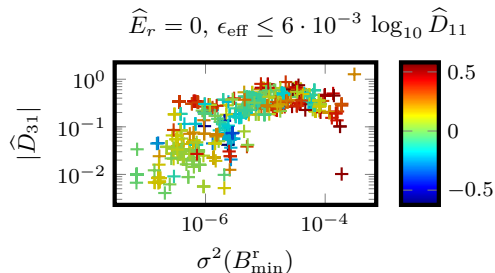


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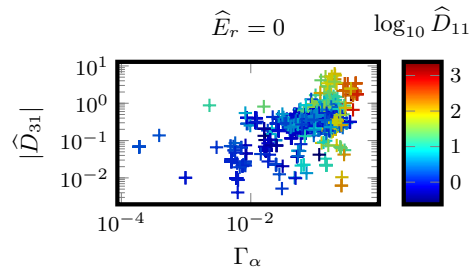
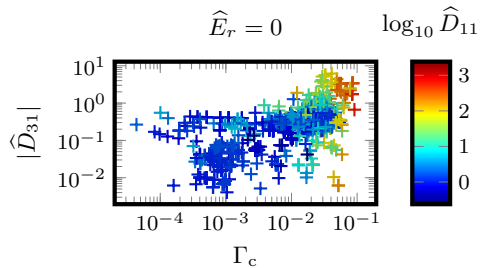
- For $\hat{E}_r = 0$ (left) minimizing the variance is inefficient. For $\sigma^2(B_{\min}^r) \sim 1 \cdot 10^{-6}$, $|\hat{D}_{31}|$ can vary almost 2 orders of magnitude.

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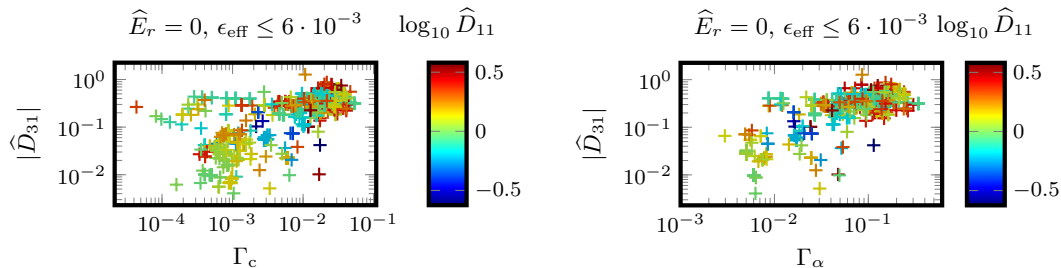


- For $\hat{E}_r = 0$ (left) minimizing the variance is inefficient. For $\sigma^2(B_{\min}^r) \sim 1 \cdot 10^{-6}$, $|\hat{D}_{31}|$ can vary almost 2 orders of magnitude.
- For $\hat{E}_r \neq 0$ (right), moderate correlation between $\sigma^2(B_{\min}^r)$ and $\hat{D}_{11}$ and between $\sigma^2(B_{\min}^r)$ and $|\hat{D}_{31}|$ is observed. Still not very efficient.

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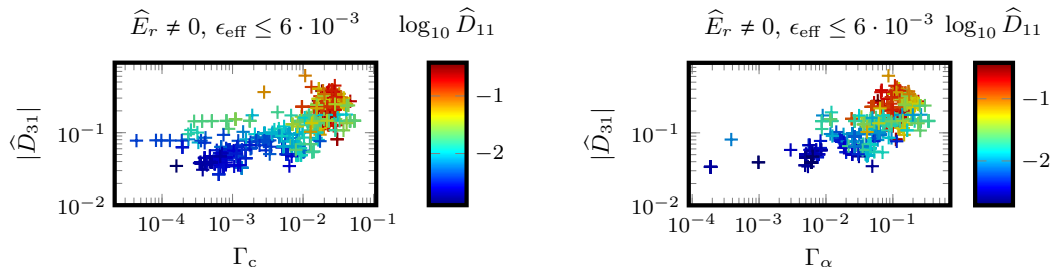


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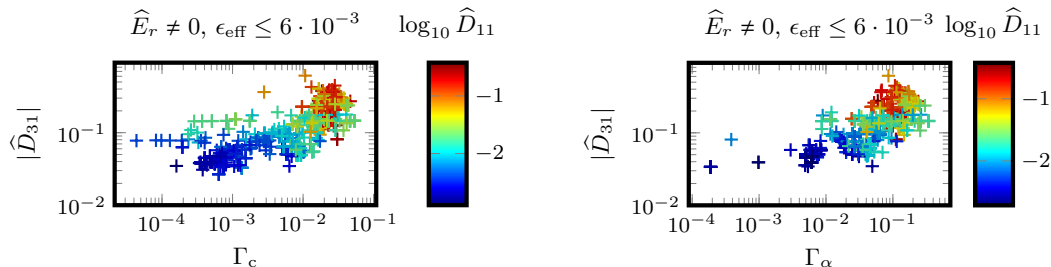
- For $\hat{E}_r = 0$, almost no correlation between Γ_c (left) and $|\hat{D}_{31}|$. Slightly better for Γ_α (right).

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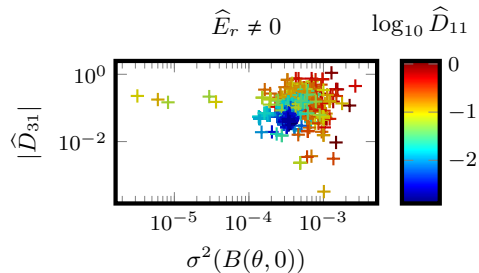
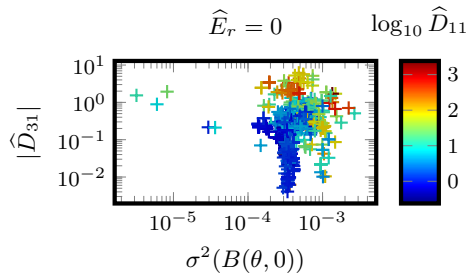
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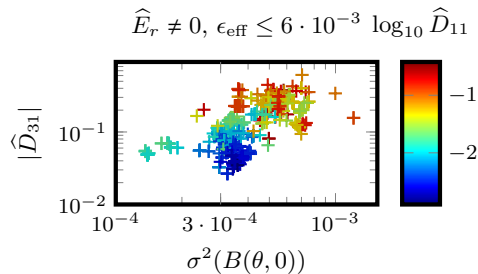
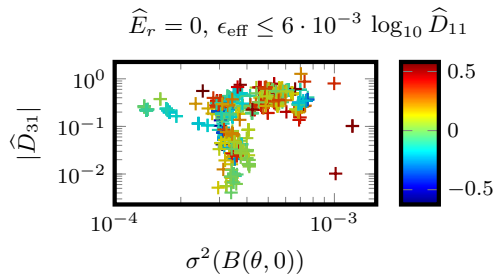
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Numerical results suggest that Γ_α allows slightly better trade-off to minimize $|\hat{D}_{31}|$ than Γ_c .

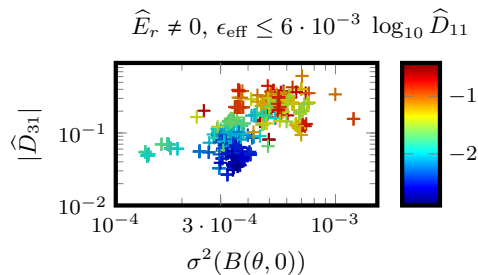
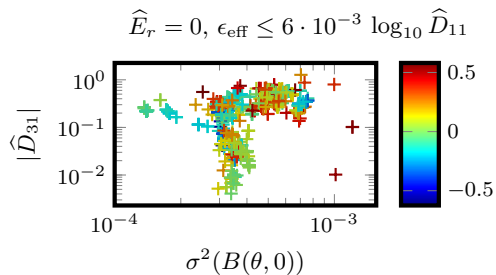
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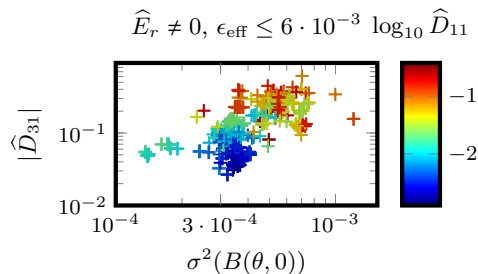
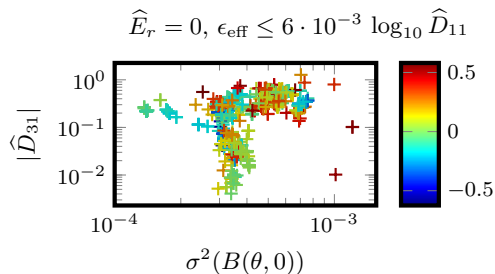


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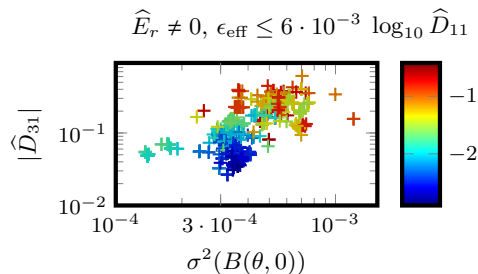
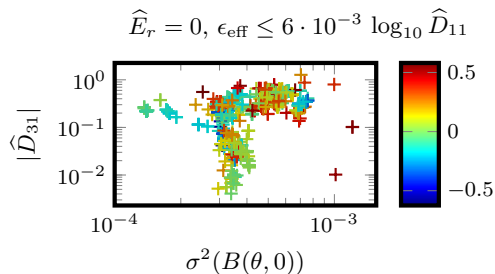
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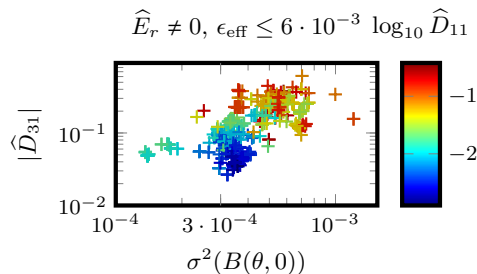
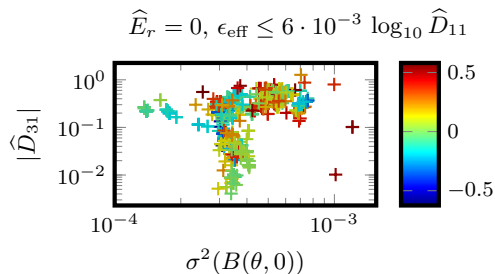
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The indirect approach is not efficient for reducing the bootstrap current, specially for $\hat{E}_r = 0$. **Can we do better?** Hopefully, **direct optimization** of the $|\hat{D}_{31}|$ coefficient will improve this efficiency.

2. Computing derivatives of $\widehat{D}_{ij}$ using MONKES

Let $\eta \in \{B_{mn}, \widehat{E}_\psi, \widehat{\nu}, \iota, B_\theta, B_\zeta, \dots\}$ be a parameter upon which the DKE depends. For gradient-based optimization methods it is useful to compute

$$\frac{\partial \widehat{D}_{ij}}{\partial \eta} = \left\langle \int_{-1}^1 s_i \frac{\partial f_j}{\partial \eta} d\xi \right\rangle + \left\langle \frac{V'}{\sqrt{g}} \int_{-1}^1 \frac{\partial}{\partial \eta} \left(\frac{\sqrt{g} s_i}{V'} \right) f_j d\xi \right\rangle.$$

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Let f_j and g_i be, respectively, the solutions to the DKE and its adjoint [Paul, JPP (2020)]

$$\begin{aligned} \mathcal{V} f_j - \hat{\nu} \mathcal{L} f_j &= s_j, \\ -\mathcal{V} g_i - \hat{\nu} \mathcal{L} g_i &= s_i, \end{aligned}$$

where $\mathcal{V} := \xi \mathbf{b} \cdot \nabla + \nabla \cdot \mathbf{b} (1 - \xi^2)/2 \partial/\partial \xi - \widehat{E}_\psi / \langle B^2 \rangle \mathbf{B} \times \nabla \psi \cdot \nabla$.

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We can compute the difficult part of $\partial \widehat{D}_{ij} / \partial \eta$ using the adjoint solution g_i as

$$\left\langle \int_{-1}^1 s_i \frac{\partial f_j}{\partial \eta} d\xi \right\rangle = \left\langle \int_{-1}^1 \frac{\partial s_j}{\partial \eta} g_i d\xi \right\rangle - \left\langle \int_{-1}^1 g_i \mathcal{V}_\eta f_j d\xi \right\rangle + \frac{\partial \hat{\nu}}{\partial \eta} \left\langle \int_{-1}^1 g_i \mathcal{L} f_j d\xi \right\rangle.$$

where $\mathcal{V}_\eta$ is the differential operator whose coefficients are the derivatives of those of $\mathcal{V}$, i.e.

$$\mathcal{V}_\eta f_j := \frac{\partial}{\partial \eta} \mathcal{V} f_j - \mathcal{V} \frac{\partial}{\partial \eta} f_j.$$

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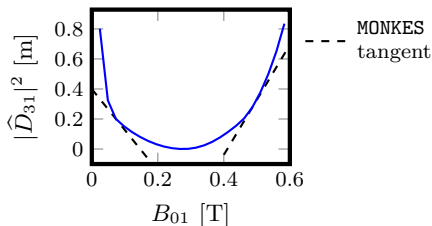
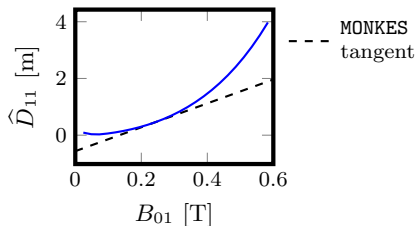
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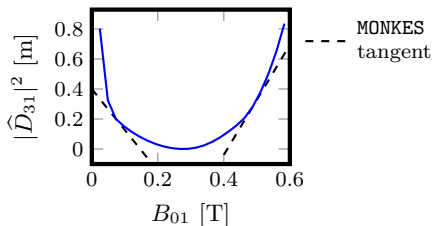
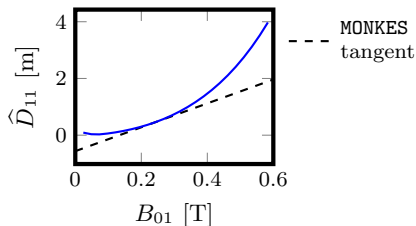


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MONKES can also provide calculations of the derivatives of the monoenergetic coefficients.

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Direct optimization of fast-ion confinement [Bindel, JPP (2023)] has inspired a new ideal design goal: piecewise omnigeneity (pwO) [Velasco, arXiv (2024)].

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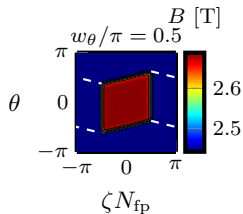
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in the limit $p \rightarrow \infty$. For $w_{\theta}/\pi > 1$, the field becomes nearly QI. Example with $p = 10$.

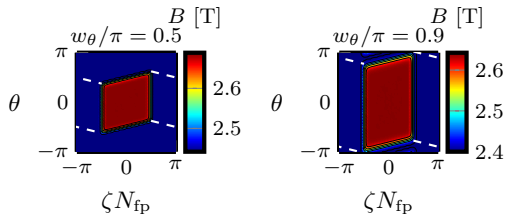


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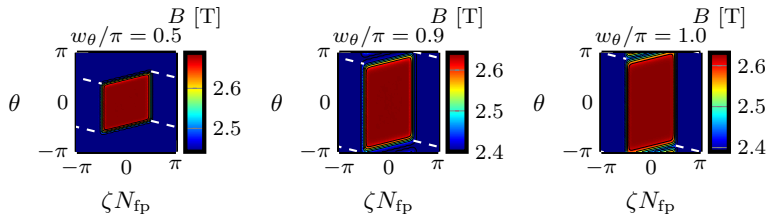


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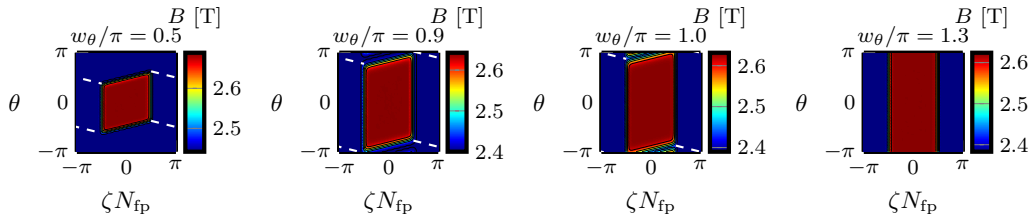


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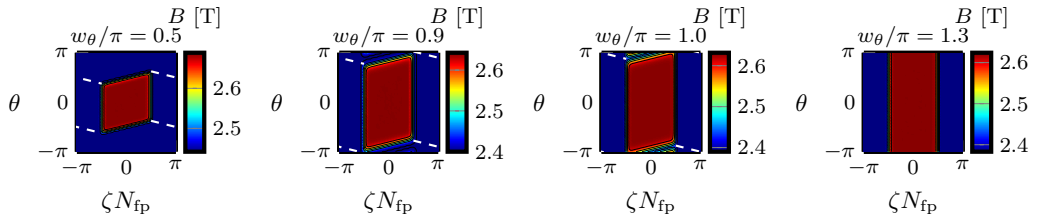


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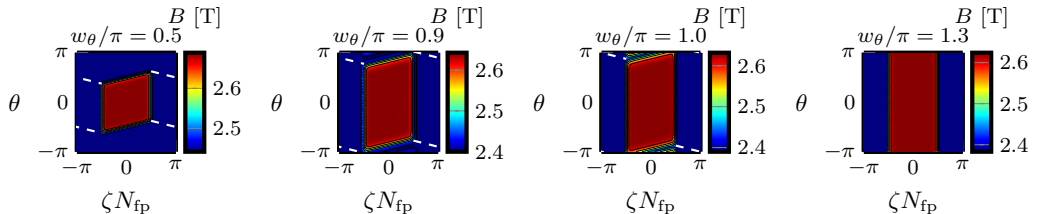
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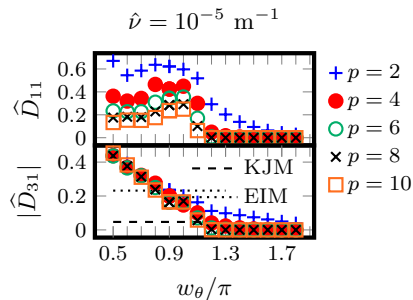
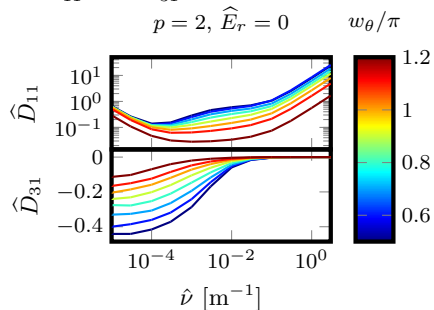
In order to identify regions of pwO parameter space with small $\hat{D}_{11}$ and $|\hat{D}_{31}|$, a scan in w_{θ} and p has been carried out. Proximity to QI is controlled by w_{θ} and proximity to pwO by p .

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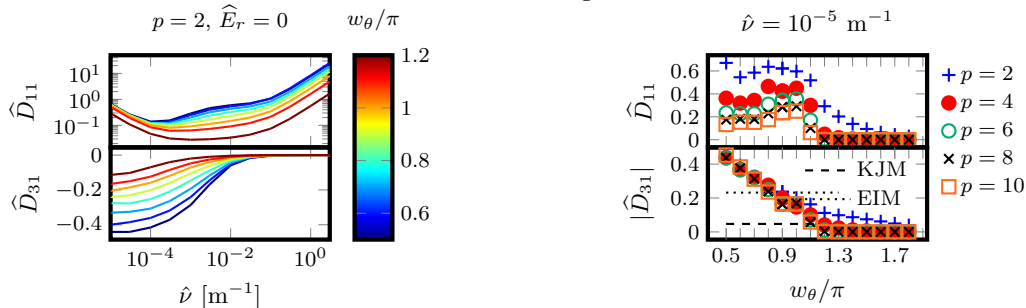
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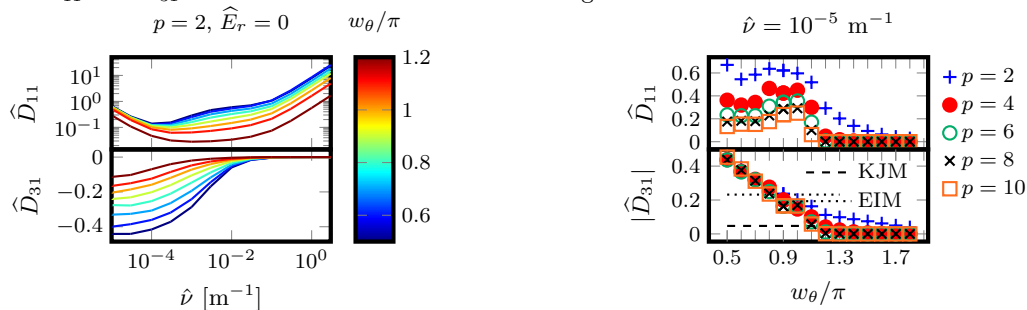
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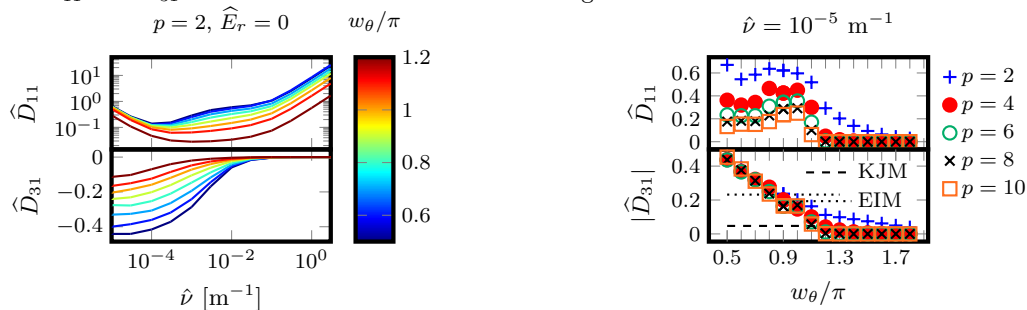
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MONKES can be used to explore extremely complicated magnetic fields. Magnetic fields can, in principle, deviate from QI to approach pwO while having low $\hat{D}_{11}$ and $|\hat{D}_{31}|$.

- ① Introduction
- ② Drift-kinetic equation and transport coefficients
- ③ Algorithm
- ④ Benchmark and code performance
- ⑤ Some applications of MONKES
- ⑥ Conclusions and future work

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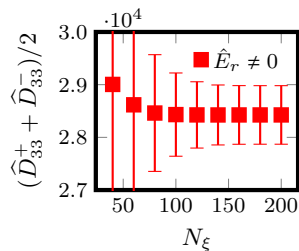
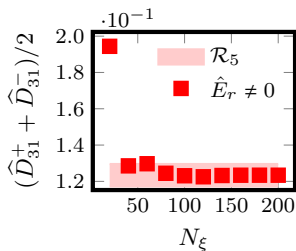
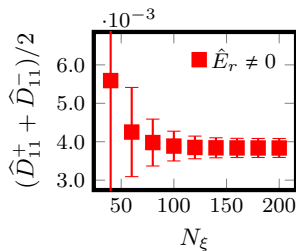
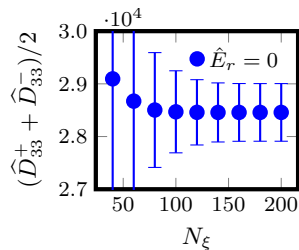
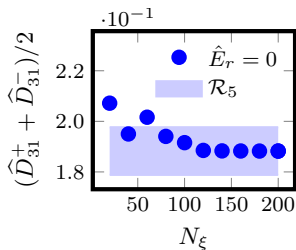
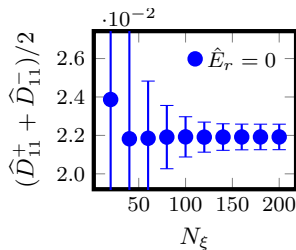
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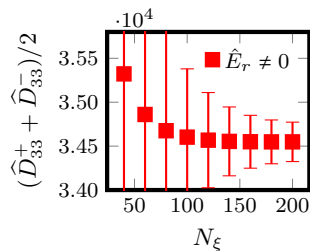
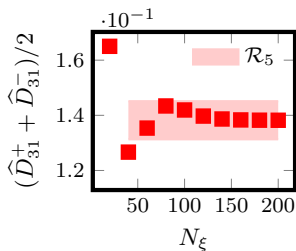
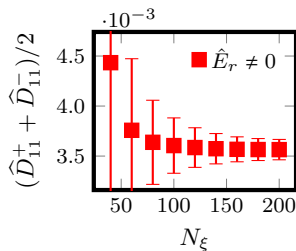
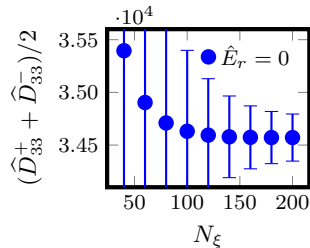
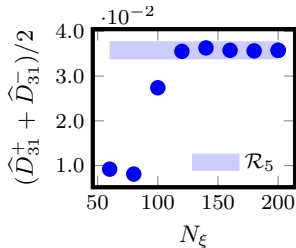
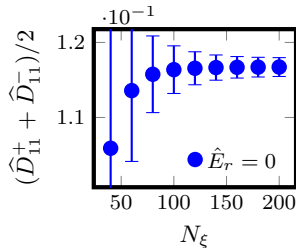
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 - Opens up the possibility of introducing the bootstrap current effect in **predictive transport simulations**.

EXTRA SLIDES

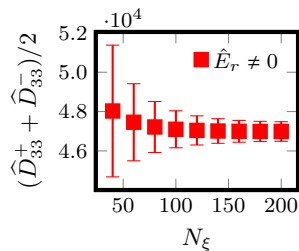
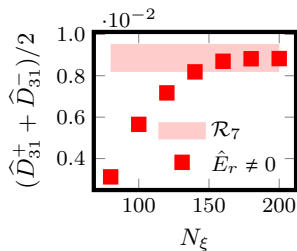
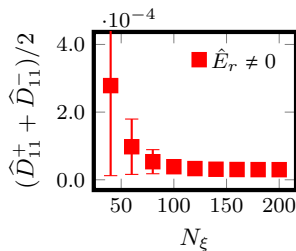
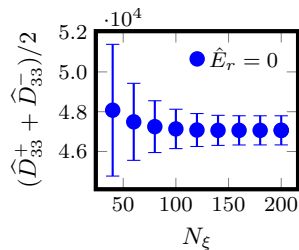
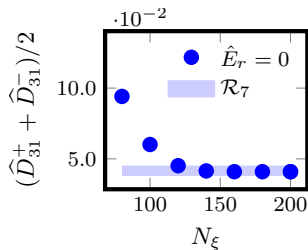
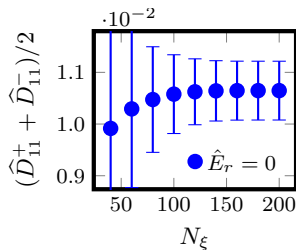
DKES convergence curves: W7-X EIM



DKES convergence curves: W7-X KJM



DKES convergence curves: CIEMAT-QI



Thermal transport coefficients

Given the monoenergetic coefficients $\hat{D}_{ij}$ as function of $\hat{\nu}(v)$ and fixed E_ψ ($\hat{E}_\psi$ can vary), we can easily calculate the thermal coefficients

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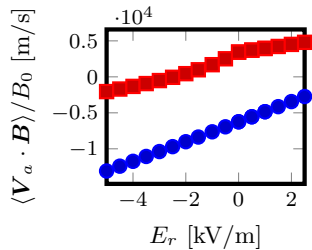
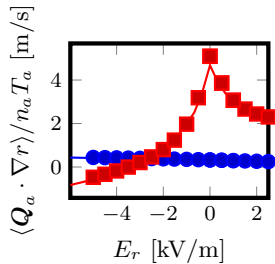
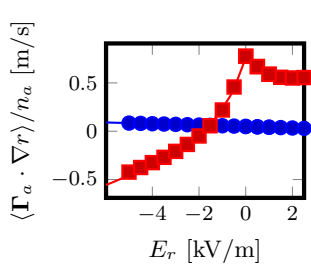
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MONKES will (soon) provide quick calculations of radial fluxes and parallel flows in multispecies stellarator plasmas.

Benchmark of neoclassical fluxes



Direct approach for computing derivatives of the transport coefficients

Suppose $\eta \in \{\hat{\nu}, \hat{E}_\psi, \{B_{mn}\}_{mn \in \mathbb{Z}}, \iota, B_\zeta, B_\theta, \dots\}$ is a parameter upon which the DKE depends. For gradient-based optimization methods (among other things) it is useful to compute

$$\frac{\partial \hat{D}_{ij}}{\partial \eta} = \left\langle \frac{1}{\sqrt{g}} \int_{-1}^1 \sqrt{g} s_i \frac{\partial f_j}{\partial \eta} d\xi \right\rangle + \left\langle \frac{1}{\sqrt{g}} \int_{-1}^1 \frac{\partial(\sqrt{g} s_i)}{\partial \eta} f_j d\xi \right\rangle.$$

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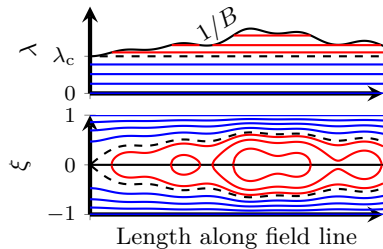
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- For $N_\eta \lesssim N_\xi N_{\text{fs}}$ the direct method is faster than an adjoint method.

Contribution of different classes of particles to $\hat{D}_{ij}$

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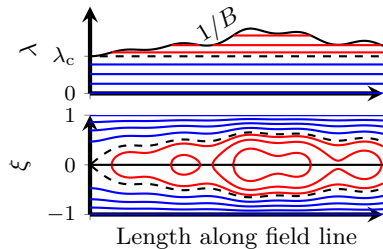


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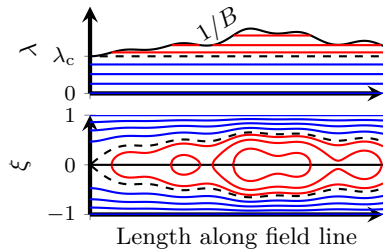
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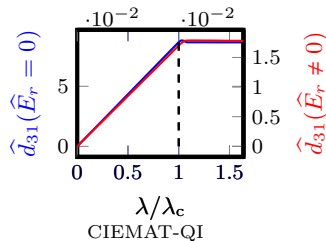
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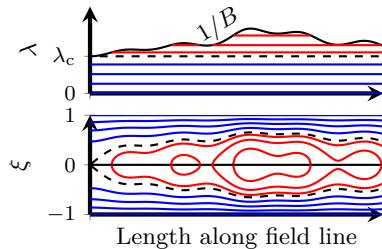


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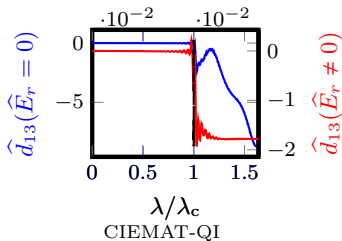
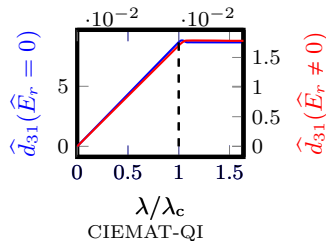
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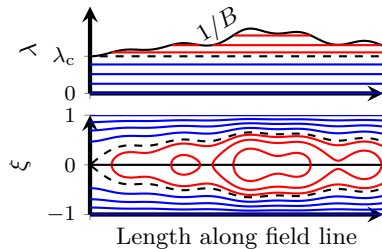


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