

Energetic particle optimization of stellarator devices using near-axis magnetic fields

Rogerio Jorge

P. Rodrigues, J. Ferreira, A. Figueiredo, R. Coelho, D. Borba, P. Figueiredo





This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Motivation

How to guarantee alpha particle heating in stellarator reactors?

How to decrease first wall damage from unconfined particles?

- Particle confinement is usually considered the Achilles Heel of stellarators
- New proxies have changed this paradigm
- Analytical models (e.g., near-axis expansion) decrease degrees of freedom but have other tradeoffs

Near axis expansion,

- The near-axis can also provide physical

insight and guide future designs



Goals



Obtain reactor relevant stellarator shapes in a reliable and efficient manner

1.3



Typical degrees of freedom to solve $J \times B = \nabla P$ - Fixed boundary (LCFS): ~100 Fourier coefficients - Free boundary (coils): ~400 Fourier coefficients

Near-axis (high aspect ratio) degrees of freedom - Axis + 1st order + 2nd order: ~10 Fourier coefficients

Is this gain worth it?

EnR Task Specification

The project is divided into 5 different tasks (WP)

- WP1 Particle tracer code development (near-axis & full MHD)
- WP2 Combine particle tracer and stellarator optimization codes
- WP3 Optimized stellarator equilibria (QS, QI and General)
- WP4 Physics study of Nemov's criterion
- WP5 Fast particle orbits in realistic magnetic fields

With the following goals

- Create an open-source, user friendly, fully tested particle tracer (WP1, WP2)
- Perform the first direct fast particle optimization of a stellarator (WP3)
- Compare fast particle optimization with commonly used proxies (WP4)
- Extend the optimization to stochastic magnetic fields (WP5)

2022

2023



Publications



First Author	Title of work	Journal	DOI
Rogerio Jorge	Single-Stage Stellarator Optimization: Combining Coils with Fixed Boundary Equilibria	Plasma Physics and Controlled Fusion, 65 074003 (2023)	doi.org/10.1088/1361- 6587/acd957
Paulo Figueiredo	Energetic Particle Tracing in Optimized Quasisymmetric Stellarator Equilibria	Journal of Plasma Physics, 90(2), 905900207 (2024)	doi.org/10.1017/S00223 77824000400
Rogerio Jorge	Direct Microstability Optimization of Stellarator Devices	Physical Review E, 110(3), 035201 (2024)	doi.org/10.1103/PhysRe vE.110.035201
Miguel Madeira	Tokamak to Stellarator Conversion using Permanent Magnets	Plasma Physics and Controlled Fusion, 66 085008 (2024)	doi.org/10.1088/1361- 6587/ad5586
Pedro Curvo	Using Deep Learning to Design High Aspect Ratio Fusion Devices	Journal of Plasma Physics (submitted)	arXiv:2409.00564
Estêvão Gomes	Differentiable Single-Stage Optimization of Stellarator Coils Based on Alpha Particle Losses	Journal of Computational Physics (in preparation)	-

EnR Task Specification



2022

The project is divided into 5 different tasks (WP)

- WP1 Particle tracer code development (near-axis & full MHD)
- WP2 Combine particle tracer and stellarator optimization codes
- WP3 Optimized stellarator equilibria (QS, QI and General)
- WP4 Physics study of near-axis expansion and Nemov's criterion 2023
- WP5 Fast particle orbits in realistic magnetic fields

With the following goals

- Create an open-source, user friendly, fully tested particle tracer (WP1, WP2)
- Perform the first direct fast particle optimization of a stellarator (WP3)
- Compare fast particle optimization with commonly used proxies (WP4)
- Extend the optimization to stochastic magnetic fields (WP5)





User-friendly example in near-axis geometry





Flexible geometries

- VMEC output files
- Near-axis analytical model
- Near-axis quasisymmetry (exact/partial)
- Dommaschk potentials (magnetic islands)

Multiple tracers

- SIMPLE
- gyronimo
- SIMSOPT
- BEAMS3D

Benchmark available on https://github.com/rogeriojorge/ particle_tracing_benchmark





NEAT is fast as it uses C++ for trajectory calculations,

which are called via Python

But can we simplify it further?

Use JAX!



JAX: High-Performance Array Computing

JAX is <u>Autograd</u> and <u>XLA</u>, brought together for high-performance numerical computing.

- JAX allows python scripts to run as fast as compiled code
- JAX provides derivatives of the output of the code with respect to the input (backpropagation)
- The same code can be run on CPUs and GPUs

Scaling with problem size Wall time per 1M grid cells (lower is better)



JAX performance compared to other compiled and parallelized backends [1]

[1] D. Hafner et al, "Fast, Cheap and Turbulent – Global Ocean Modeling with GPU Acceleration in Python, Journal of Advances in Modeling Earth Systems 13 (2021)



Particle tracer code ESSOS using:

- only Python
- hybrid OpenMP/MPI parallelization
- able to run on CPUs and GPUs



Guiding Center Equations

On Biot-Savart coil fields

Developed by IST undergrad Student



Estêvão Moreira Gomes

EstevaoMGomes

Pinned

uwplasma/ESSOS Public

Estêvão's Single Stage Optimizer of alpha particles via differentiable JAX code

Python

54 contributions in the last year



Optimized stellarator (WP5)





Particle tracer code ESSOS using:

- only Python
- hybrid OpenMP/MPI parallelization
- able to run on CPUs and GPUs

Developed by IST undergrad Student



Estêvão Moreira Gomes

EstevaoMGomes

Pinned

uwplasma/ESSOS Public

Estêvão's Single Stage Optimizer of alpha particles via differentiable JAX code

Python

54 contributions in the last year



Benchmarks





EnR Task Specification



2022

The project is divided into 5 different tasks (WP)

- WP1 Particle tracer code development (near-axis & full MHD)
- WP2 Combine particle tracer and stellarator optimization codes
- WP3 Optimized stellarator equilibria (QS, QI and General)
- WP4 Physics study of near-axis expansion and Nemov's criterion 2023
- WP5 Fast particle orbits in realistic magnetic fields

With the following goals

- Create an open-source, user friendly, fully tested particle tracer (WP1, WP2)
- Perform the first direct fast particle optimization of a stellarator (WP3)
- Compare fast particle optimization with commonly used proxies (WP4)
- Extend the optimization to stochastic magnetic fields (WP5)

WP2 – Combine particle tracer and stellarator optimization codes



2. Integration with stellarator optimization frameworks (WP2)

- scipy.optimize.minimize or SIMSOPT near-axis
- SIMSOPT full MHD
 DESC full MHD (finalizing)



EnR Task Specification



- 2022

The project is divided into 5 different tasks (WP)

- WP1 Particle tracer code development (near-axis & full MHD)
- WP2 Combine particle tracer and stellarator optimization codes
- WP3 Optimized stellarator equilibria (QS, QI and General)
- WP4 Physics study of near-axis expansion and Nemov's criterion 2023
- WP5 Fast particle orbits in realistic magnetic fields

With the following goals

- Create an open-source, user friendly, fully tested particle tracer (WP1, WP2)
- Perform the first direct fast particle optimization of a stellarator (WP3)
- Compare fast particle optimization with commonly used proxies (WP4)
- Extend the optimization to stochastic magnetic fields (WP5)

Each point takes ~1 second on a laptop -0.20 -0.15 -0.10 -0.050.00 0.05 0.10 RBC(1.0) Rogerio Jorge | EUROfusion Science Meeting | Results of Enabling Research Projects 2021-2024 | October 23, 2024

WP3 – Optimized stellarator equilibria



14

- 3. Optimized stellarator configurations (WP3)
 - Obtained Near-Axis Optimizations (previous slide)
 - Obtained full MHD Optimizations

Minimal benchmark problem

- Trace 2400 particles for 5×10^{-4} s with the SIMPLE code
- Scale the minor radius and magnetic field to half of the **ARIES-CS** reactor
- Save the fraction of loss particles in an array for each **RBC(1,0)**







Scripts available on https://github.com/rogeriojorge/EPoptimization

- 3. Optimized stellarator configurations (WP3)
 - Obtained Near-Axis Optimizations (previous slide)
 - Obtained full MHD Optimizations







16

Focus on the near-axis expansion

 Viability of near-axis solutions as good initial conditions for full MHD designs

P. A. Figueiredo et al, JPP Volume 90, Issue 2, April 2024



• Near-axis database and machine learning model

J. Candido, Undergraduate Thesis (2022/2023) P. Curvo, Undergraduate Thesis (2023/2024) – submitted to JPP

J / PICNeuralNetworkQuasisymmetricStellara Q Type[] to search	E C pedrocurvo / MLStellaratorDesign Δ Q Type () to search
<> Code 😳 Issues 11 Pull requests 🕑 Actions 🖽 Projects 🛈 Security 🗠 Insights	Scode ⊙ Issues the Pull requests ♀ Discussions ⊙ Actions Projects Wiki
Se PICNeuralNetworkQuasisymmetricStellarator (Public)	MLStellaratorDesign Private O Unwatch 2
[1 ² main → 1 ² 4 Branches ⊗ 0 Tags Q. Go to file € + ↔ Code →	P main → P 1Branch ⊗ 0 Tags Q Go to file € + ◆ Code →
😪 JoaoAGCandido results: mae mse std b3fb680 · 8 months ago 🕥 135 Commits	🛞 diogoff untracking .gitattributes 9d3d0ad - 9 hours ago 🕥 79 Commits



P. Curvo, D. R. Ferreira, R. Jorge



Focus on the near-axis expansion

Create near-axis plasma boundaries and export them to VMEC. Viability of near-axis solutions as good initial Compare (R, Z) values of a near-axis vs. VMEC point conditions for full MHD designs P. A. Figueiredo et al, JPP Volume 90, Issue 2, April 2024 aspect ratio = 6.51aspect ratio = 8.26aspect ratio = 10.53 10^{-1} Relative Error in Location Ν C N $^{-1}$ 10^{-2} R aspect ratio = 13.46aspect ratio = 17.23aspect ratio = 22.072 10^{-3} (RaxisvMEC - Raxisnear - axis)/RaxisvMEC (Zaxisvmec – Zaxisnear – axis)/Zaxisvmec $(R_{VMEC} - R_{near-axis})/R_{VMEC}$ Ν Ν Ν $(Z_{VMEC} - Z_{near - axis})/Z_{VMEC}$ $(\iota_{VMEC} - \iota_{near-axis})/\iota_{VMEC}$ -1 Initial flux surface 2×10^{1} 10^{1} -2 Aspect Ratio of the Plasma Boundary Near-Axis (tဋ្ဌue) agis 9 VMEC Initial Position R R Near-Axis (true) Initial Position



Focus on the near-axis expansion

Viability of near-axis solutions as good initial conditions for full MHD designs

P. A. Figueiredo et al, JPP Volume 90, Issue 2, April 2024

Use NEAT to benchmark codes (gyronimo vs SIMPLE)



FIGURE 3. Orbits obtained with SIMPLE with $(s, \theta, \phi) = (0.25, 2.89, 1.84)$ and $v_{\parallel}/v = 0.44$ as



qyronimo and SIMPLE tracers for original precise QA, scaled to A and B_0 , the field at the plasma axis. With an initial position

Rogerio Jorge | EUROfusion Science Meeting | Results of Enabling Research Projects 2021-2024 | October 23, 2024 18

Physics



Focus on the near-axis expansion

 Viability of near-axis solutions as good initial conditions for full MHD designs

P. A. Figueiredo et al, JPP Volume 90, Issue 2, April 2024

- 1. Use NEAT to benchmark codes
- 2. Compare near-axis vs. full MHD orbits







Journal of Plasma Physics

rticle	Figu	res Met	rics		
🔒 Save I	PDF	A Share	66 Cite	Rights & Permissions	





Focus on the near-axis expansion

 Viability of near-axis solutions as good initial conditions for full MHD designs

P. A. Figueiredo et al, JPP Volume 90, Issue 2, April 2024

- 1. Use NEAT to benchmark codes
- 2. Compare near-axis vs. full MHD orbits
- 3. Compare near-axis vs full MHD loss fractions









Focus on the near-axis expansion

 Viability of near-axis solutions as good initial conditions for full MHD designs

P. A. Figueiredo et al, JPP Volume 90, Issue 2, April 2024

- 1. Use NEAT to benchmark codes
- 2. Compare near-axis vs. full MHD orbits
- 3. Compare near-axis vs full MHD loss fractions
- 4. Obtain analytical formulas for the trapped-passing boundary and banana width using near-axis expansion

$$\frac{(1+a_A\sqrt{s_i}\ \bar{\eta}\cos\theta_i)}{(1+a_A\sqrt{s_i+2\Delta s}\ |\bar{\eta}|)} \leqslant \lambda_s \leqslant \frac{(1+a_A\sqrt{s_i}\ \bar{\eta}\cos\theta_i)}{(1+a_A\sqrt{s_i-2\Delta s}\ |\bar{\eta}|)}$$

 $\Delta s = \frac{mvL\bar{\eta}}{\pi q \ \iota_{N_0} a_A B_0} \frac{1 - \lambda B_0 / (2B_i)}{\sqrt{1 - \lambda B_0 / B_i}} \left(2\sqrt{s_i} + \left(\sqrt{s_i + \Delta s_{avg}} - \sqrt{s_i}\right) \cos \theta_i \right)$



ournal of Plasma

Physics









22

Focus on the near-axis expansion

• Near-axis database and machine learning model J. Candido, Undergraduate Thesis (2022/2023) P. Curvo, Undergraduate Thesis (2023/2024)

1. Create a near-axis database similar to M. Landreman, JPP 88(6), 2022







Focus on the near-axis expansion

• Near-axis database and machine learning model J. Candido, Undergraduate Thesis (2022/2023) P. Curvo, Undergraduate Thesis (2023/2024)

J / PICNeuralNetworkQuasisymmetricStellara Q. Type [] to search	E pedrocurvo / MLStellaratorDesign & Q. Type [] to sea	Q. Type [] to search	
↔ Code 💿 Issues 🏦 Pull requests ⊙ Actions 🗄 Projects 💮 Security 🗠 Insights	↔ Code ⓒ Issues th Pull requests © Discussions ⓒ Actions 🗄 P	rojects 🖽 Wiki	
September 2 - O Unwatch 2 -	MLStellaratorDesign (Private)	⊙ Unwatch 2	
P main → P 4 Branches ⊗ 0 Tags: Q. Go to file (t) + 🗘 Code →	[1 main •] 14 Branch (\$ 0 Tags (Q. Go to file (*)	F 🔷 Code 🕞	
📚 JoaoAGCandido results: mae mse std b3tb680 · 8 months ago 🕥 135 Commits	🛞 diogoff untracking .gitattributes 9d3d0ad - 9 hours ago	🕚 79 Commits	

- 1. Create a near-axis database similar to M. Landreman, JPP 88(6), 2022
- 2. Experiment with data-reduction and clustering methods (e.g., find division between QA and QH)





Focus on the near-axis expansion

• Near-axis database and machine learning model J. Candido, Undergraduate Thesis (2022/2023) P. Curvo, Undergraduate Thesis (2023/2024)

- 1. Create a near-axis database similar to M. Landreman, JPP 88(6), 2022
- 2. Experiment with data-reduction and clustering methods (e.g., find division between QA and QH)
- 3. Train neural network to reproduce forward and inverse solutions

Forward model (easy to reproduce)

	Adjusted R-Squared	R–Squared	RMSE	Time Taken
Model				
ExtraTreesRegressor	0.66	0.66	0.60	3.84
RandomForestRegressor	0.64	0.64	0.62	11.98
XGBRegressor	0.64	0.64	0.62	4.36
BaggingRegressor	0.61	0.61	0.64	1.21
MLPRegressor	0.59	0.59	0.65	3.54
KNeighborsRegressor	0.51	0.51	0.72	0.18
DecisionTreeRegressor	0.29	0.29	0.87	0.20
ExtraTreeRegressor	0.24	0.24	0.90	0.04
RidgeCV	0.04	0.04	0.99	0.01
Ridge	0.04	0.04	0.99	0.01
Lars	0.04	0.04	0.99	0.01
TransformedTargetRegressor	0.04	0.04	0.99	0.01
LinearRegression	0.04	0.04	0.99	0.01
KernelRidge	0.04	0.04	0.99	12.93
OrthogonalMatchingPursuit	0.04	0.04	0.99	0.01
ElasticNet	-0.00	-0.00	1.01	0.01
Lasso	-0.00	-0.00	1.01	0.01
DummyRegressor	-0.00	-0.00	1.01	0.01
LassoLars	-0.00	-0.00	1.01	0.01



Rogerio Jorge | EUROfusion Science Meeting | Results of Enabling Research Projects 2021-2024 | October 23, 2024

C J / PICNeuralNetworkQuasisymmetricStellara Q Type () to search	E O pedrocurvo / MLStellaratorDesign A Q Type () to search	
🖒 Code 💿 Issues 🏗 Pull requests 💿 Actions 🗄 Projects 💿 Security 🗠 Insights	↔ Code ⓒ Issues th Pull requests 🖓 Discussions ⓒ Actions 🗄 Projects	🛱 Wiki
Se PICNeuralNetworkQuasisymmetricStellarator (Public) (© Unwatch (2) +	MLStellaratorDesign (Private) Out	watch 2
P main - P 4 Branches © 0 Tags Q. Go to file (t) + 🗘 Code -	17 main + 17 1Branch © 0 Tags Q. Go to file 🕚 + 🔿	Code 👻
📚 JoaoAGCandido results: mae mse std b3fb680 - 8 months ago 🕥 136 Commits	diogoff untracking .gitattributes 9d3d0ad · 9 hours ago ③ 79 Co	mmits

alpha = 7.91e- 05, batch_size = 87, hidden_layer_sizes = [45, 45, 45, 45], learning_rate_init = 9.3×10^{-4}

24



25

Focus on the near-axis expansion

Near-axis database and machine learning model J. Candido, Undergraduate Thesis (2022/2023) P. Curvo, Undergraduate Thesis (2023/2024)

- Create a near-axis database similar to M. Landreman, JPP 88(6), 2022
- Experiment with data-reduction and clustering methods (e.g., find division between QA and QH)

P 4 Branches 0 0 Tags

JoaoAGCandido results: mae mse std

- 3. Train neural network to reproduce forward and inverse solutions
- Train mixture density networks to solve the inverse design problem 4.





EnR Task Specification



- 2022

The project is divided into 5 different tasks (WP)

- WP1 Particle tracer code development (near-axis & full MHD)
- WP2 Combine particle tracer and stellarator optimization codes
- WP3 Optimized stellarator equilibria (QS, QI and General)
- WP4 Physics study of near-axis expansion and Nemov's criterion ~ 2023
- WP5 Fast particle orbits in realistic magnetic fields

With the following goals

- Create an open-source, user friendly, fully tested particle tracer (WP1, WP2)
- Perform the first direct fast particle optimization of a stellarator (WP3)
- Compare fast particle optimization with commonly used proxies (WP4)
- Extend the optimization to stochastic magnetic fields (WP5)

Physics study of Nemov's criterion



Nemov Γ_c - minimize radial drift of trapped orbits

$$\Gamma_{c} = \frac{\pi}{\sqrt{B}} \lim_{L \to \infty} \left(\int_{0}^{L} \frac{dI}{B} \right)^{-1} \int_{1}^{B_{max} / B_{min}} db' \qquad V_{r} \text{ - bounce average radial drift } \frac{\partial J}{\partial \alpha} \\ \times \sum_{well_{j}} V_{c}^{2} \frac{v\tau_{b,j}}{4B_{min} b'^{2}}; \quad V_{c} = \frac{2}{\pi} \arctan \frac{v_{r}}{v_{\theta}} \qquad J = \int_{bounce} \sqrt{1 - \frac{|B|}{b'}} dl \text{ - adiabatic invariant}$$

Higher resolution and longer field lines create discontinuities between wells leading to noise



Many turning points on unoptimized stellarators make calculation very complex



Calculate J at each surface and normalized magnetic moment $b'=1/\lambda$ by bounce averaging



EnR Task Specification



- 2022

The project is divided into 5 different tasks (WP)

- WP1 Particle tracer code development (near-axis & full MHD)
- WP2 Combine particle tracer and stellarator optimization codes
- WP3 Optimized stellarator equilibria (QS, QI and General)
- WP4 Physics study of near-axis expansion and Nemov's criterion 2023
- WP5 Fast particle orbits in realistic magnetic fields

With the following goals

- Create an open-source, user friendly, fully tested particle tracer (WP1, WP2)
- Perform the first direct fast particle optimization of a stellarator (WP3)
- Compare fast particle optimization with commonly used proxies (WP4)
- Extend the optimization to stochastic magnetic fields (WP5)

WP5 – Fast particle orbits in realistic magnetic fields



Implementation of particle tracing on DESC (collaboration with PPPL)



Stellarator Optimization Package

😡 license MIT DOI 10.5281/zenodo.4876504 issues 73 open pypi v0.1

🔢 docs passing 💭 Unit tests passing 💭 Regression tests passing 🌳 codecov 95%

- Summer 2023 visit of João Biu to Princeton
- Particle tracing now implemented in DESC
- DESC uses automatic differentiation
 - Study of direct particle tracing using automatic differentiation underway



Rogerio Jorge | EUROfusion Science Meeting | Results of Enabling Research Projects 2021-2024 October 23, 2024

29

WP5 – Fast particle orbits in realistic magnetic fields





Rogerio Jorge | EUROfusion Science Meeting | Results of Enabling Research Projects 2021-2024 | October 23, 2024

30

End

