TSVV-12:
Stellarator Optimization

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1 IPP, 2 Aalto University, 3 TU Graz, 4 EPFL, (5 PPPL,) 6 CIEMAT

EUROfusion Science Meeting | 11-12 of Sept. 2023

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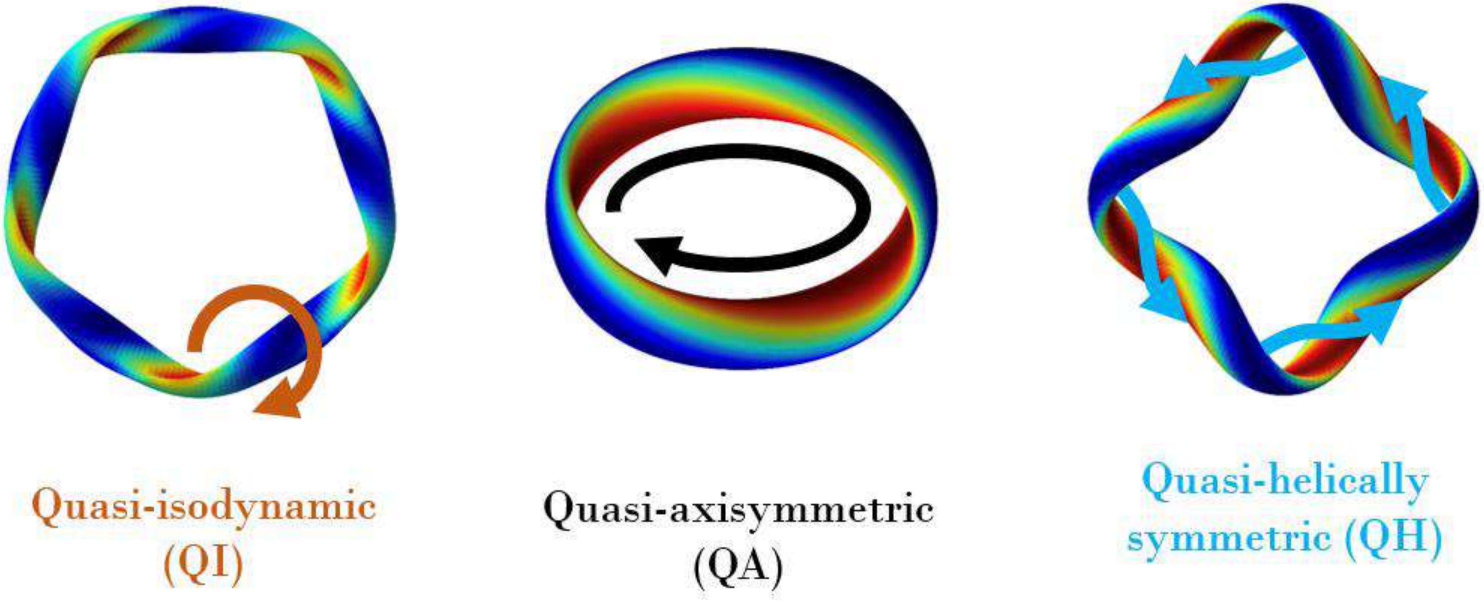
Content

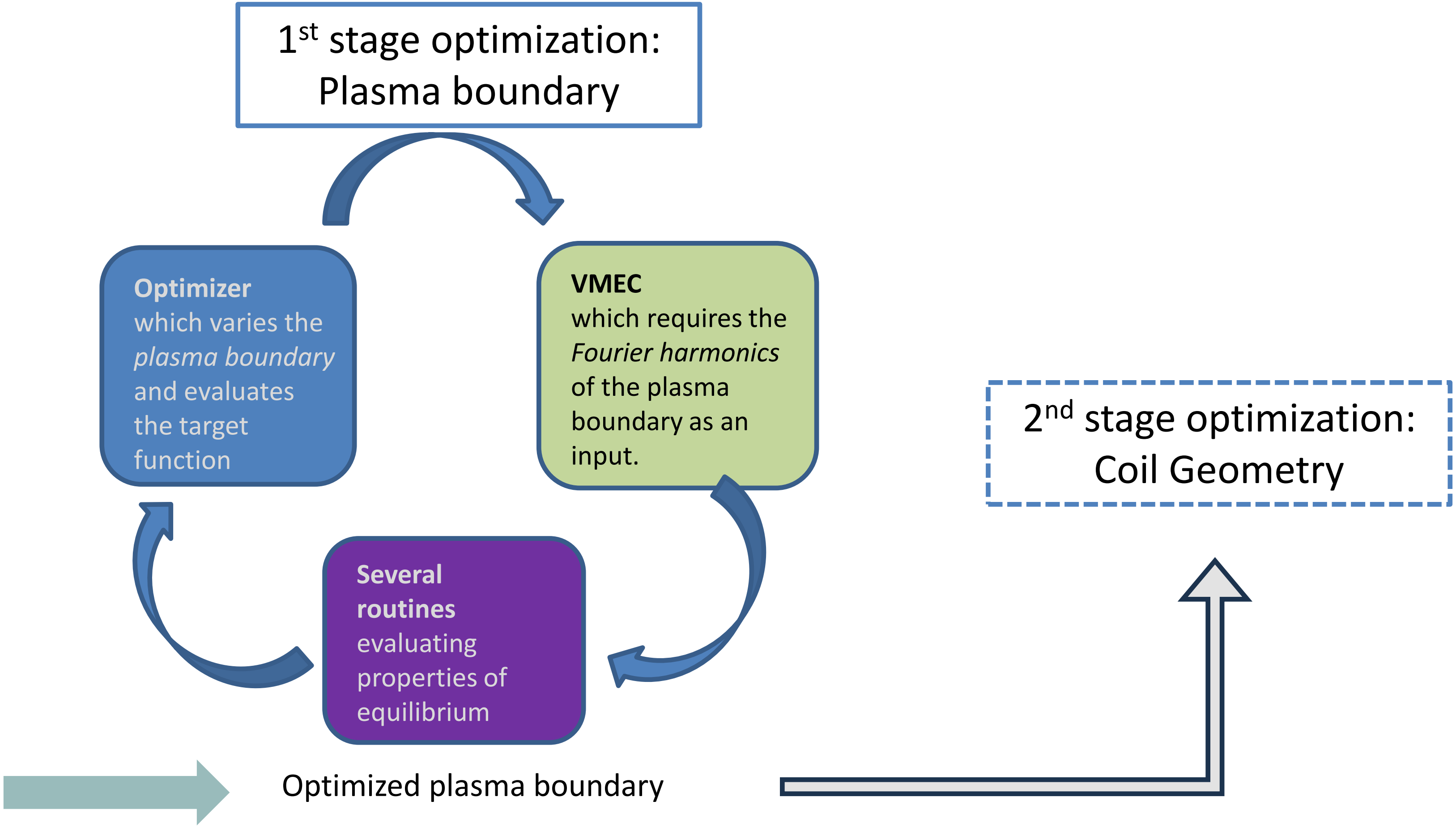
- Background on Stellarator (Optimization)
- Overview of our collaboration
  - Goals of our collaboration
  - Introduction of our team
  - Overview of progress
- Selected Research Highlights
  - New tools & better understanding
  - 3 new stellarator designs
- Summary & remaining goals

Hidden symmetries

- Perfect collisionless orbit confinement requires all level curves of **|B|** on each flux surface to have the same topology.
- Three possibilities:



Traditional approach in Stellarator Optimization



1st stage optimization:
Plasma boundary

Optimizer
which varies the *plasma boundary* and evaluates the target function

VMEC
which requires the *Fourier harmonics* of the plasma boundary as an input.

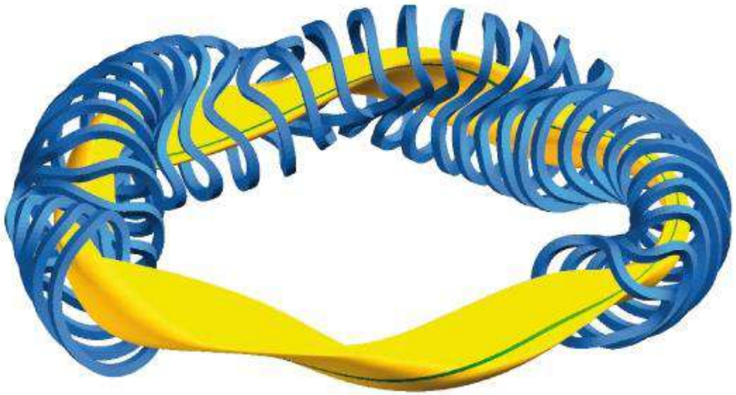
Several routines
evaluating properties of equilibrium

Optimized plasma boundary

2nd stage optimization:
Coil Geometry

Stellarator Optimization

- W7-X works very well e.g. Beidler et al. Nature (2021)
- But W7-X could (and should!) be improved in a few ways:
  - Fast-ion confinement
  - Turbulence
  - Coils
  - Divertor



W7-X plasma boundary surface and modular coils

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Key Deliverables of our team

1. Turbulent & Neoclassical Transport: *Integration of fast reduced models of turbulent transport into stellarator optimization codes (synergy with TSVV Task 13) Generalization of tools for the evaluation of radial neoclassical transport, so that it can be minimized in collisionality regimes beyond the 1/n regime*.
2. Bootstrap Current & Energetic Particle Confinement: *Accurate numerical tools for the evaluation of energetic particle confinement and for the calculation of the bootstrap current that are sufficiently fast to be integrated into stellarator optimization code.*
3. MHD equilibrium and stability: *Efficient tools capable of assessing, for any stellarator equilibrium, ideal and resistive MHD stability (and the importance thereof), and robustness of the magnetic topology to current perturbations.*
4. Improved optimization approaches: *Improved algorithms to be employed in stellarator optimization for reduced sensitivity to local optima in parameter space, and development of approaches for coil simplification and robustness against errors.*
5. Stellarator Optimization: *Application to produce a set of highly optimized stellarator configurations.*
6. Power Exhaust: *Investigation on the integration of power options for next-generation stellarators*.

Our team – wide range of expertise

- **IPP** (Per Helander (**PI**), Sophia Henneberg (**deputy PI**), Michael Drevlak, Gabriel Plunk, Samuel Lazerson, Carolin Nührenberg, Yuhe Feng, Brendan Shanahan, Omar Maj, Florian Hindenlang, Alan Goodman, Brandon Lee, Craig Beidler, Gareth Roberg-Clark, Robert Davies, Tiago Ribeiro)
- **CIEMAT** (Edilberto Sánchez, José Luis Velasco, Javier Escoto, Guillermo Godino, Ivan Calvo)
- **Fusion ÖAW, ITPcp, TU Graz** (Winfried Kernbichler, Sergei Kasilov, Christopher Albert)
- **Aalto University** (Simppa Äkäslompolo)
- **EPFL** (Joaquim Loizu, (Antoine Baillod), Erol Balkovic, Chirstopher Smiet)
- (**Princeton University, PPPL** (Félix Parra))

Unfunded team members
Joined team (part of TSVV email list)
+ many more collaborators

Our team – wide range of expertise

- Stellarator Optimization (with ROSE, STELLOPT and SIMSOPT)
- MHD Equilibrium and Stability (ideal & MRxMHD)
- Turbulence & Micro-Instabilities
- Neoclassical Transport
- Fast particle confinement
- Plasma Edge and Stellarator Divertors

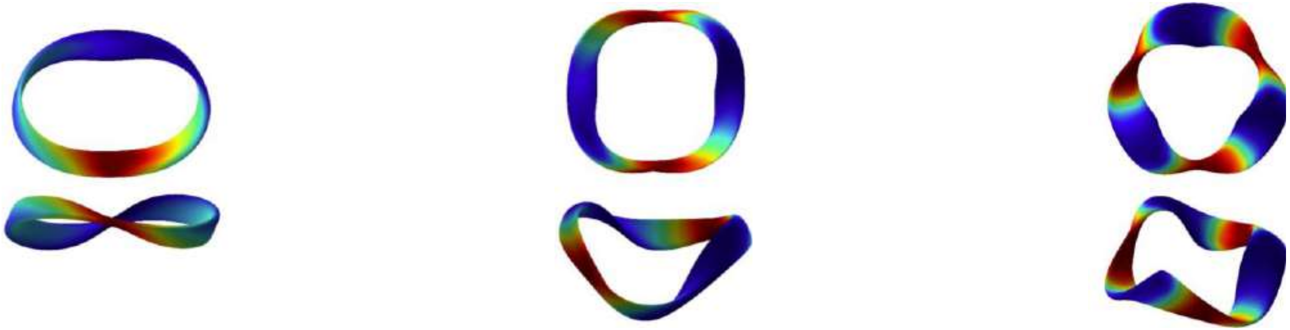
Aalto University TU Graz EPFL Ciemat MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK

Overview of promised Milestones

	Milestones promised until now:	Anticipated by	Status
SD1.2	derivation of turbulence model	the end of 2021	Achieved
SD2.2	Define and implement common interfaces for particle codes and perform cross-code validation of existing and new code parts	mid of 2023	Achieved
SD3.1	evaluate the ideal and resistive, internal and external, stability of stellarator equilibria	the end of 2021	Achieved
SD3.2	Application of different measures of departure from integrability of the magnetic field in SPEC equilibria.	the end of 2022	Achieved
SD3.4	Including CAS3D in ROSE.	the end of 2022	Achieved
SD4.3	Investigation how choice of poloidal angle influences stellarator optimization outcome	the end of 2021	Achieved
SD5.1	Implementing flexibiliy in choice of optimizer in ROSE	the end of 2021	Achieved
SD6.1	Development and use of BOUT++ simulations in stellarator geometries.	the end of 2022	Achieved

Overview of promised Milestones

New stellarator designs	Type	Publications
CIEMAT QI	QI	E. Sánchez, J. Velasco, I. Calvo, and S. Mulas, Nuclear Fusion 63, 066037 (2023)
Precise QI	**QI**	**A. Goodman, et al., “Constructing precisely quasi-isodynamic magnetic fields”, accepted JPP, arXiv:2211.09829**
QSTK	QH	G.T. Roberg-Clark, et al., “Critical gradient turbulence optimization toward a compact stellarator reactor concept”, PRR (2023)
Hybrid	QA-tokamak	S.A. Henneberg, G.G. Plunk, “A compact stellarator-tokamak hybrid”, EUROfusion IDs 354444, 36001



ACH support & Codes overview

- Several codes benefitted from ACH support:
  - GVEC: MPI parallelization
  - VM2MAG (M. Borchardt, M. Drevlak) improved for better parallel scaling.
  - CAS3D ideal-MHD-stability code was ported to GPU usage.
  - KNOSOS was optimized to be faster.
  - ASCOT5 was ported to GPU usage.
- New interfaces between codes & IMAS:
  - VMEC interfaced to IMAS via iWrap; (*With technical support by ACH*).
  - Work is underway to extend to the IMAS interface BEAMS3D and ASCOT5 (*Also with technical support by ACH*).
  - GVEC (converter to VMEC files; interface linked to GENE-3D (TSVV-13); converter for CASTOR3D & JOREK-3D)
  - SPEC, CAS3D and KNOSOS coupled into optimization suites
- Validation & Verification efforts
  - Validation activities for KNOSOS have been performed in collaboration with the W7-X team.
  - A verification activity comparing ASCOT5, BEAMS3D, ANTS, and VENUS-LEVIS has been carried out. Benchmarking for neutral beam deposition has been performed.
  - Work is ongoing to benchmark BEAMS3D against ASDEX-U and W7-X data using a newly developed FIDASIM interface (developed under the EnR on Phase Space Tomography, Moseev).
  - Introducing uncertainty quantification to 3D MHD equilibrium computation [R. Köberl, et al, *Contrib. To Plasma Phys,* 2023]

ACH support & Codes overview

- Additional relationships to other projects:
  - CIEMAT: TSVV13 (regarding turbulent transport), WPW7X
  - SPEC: TSVV-3, EnR project of University of Lisbon
  - KNOSOS has been applied to experimental studies within WPW7X
  - Guiding-center tracers SIMPLE and GORILLA used in TSVV12 and TSVV6, respectively benefited from benchmarking and joint development
  - Simons collaboration
  - HILOADS collaboration
- The STELLOPT family of codes (VMEC, BEAMS3D, FIELDLINES, DIAGNO, STELLOPT, NEO, DKES, etc.) is documented under the VMECwiki. The STELLOPT family of codes is freely available under a MIT License and is maintained on GitHub. *https://github.com/PrincetonUniversity/STELLOPT*
- Documentation of the CAS3D, SIMPE and GVEC code is being implemented as part of the GIT repository.
  - https://gitlab.mpcdf.mpg.de/cas/cas3d
  - https://github.com/itpplasma/SIMPLE
  - https://gitlab.mpcdf.mpg.de/gvec-group/gvec
- BOUT++ is completely open source on github: https://github.com/boutproject/bout-dev

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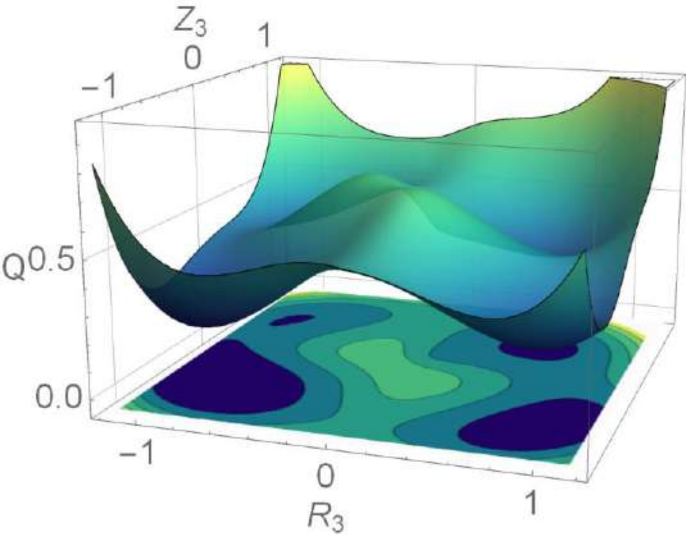
Unique plasma boundary representation

S.A. Henneberg, P. Helander, M.Drevlak, J. Plasma Phys. (2021)

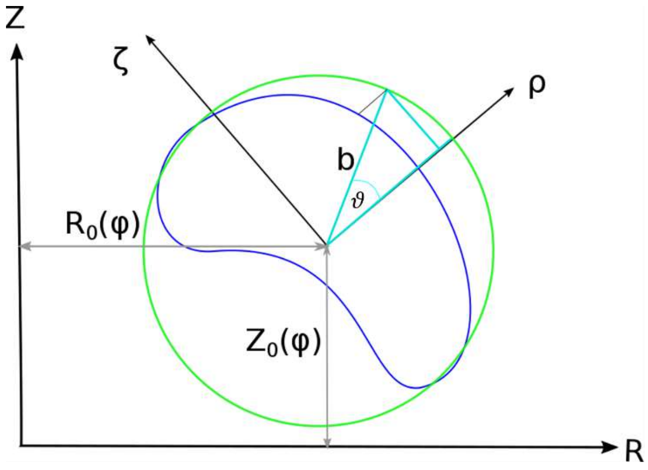


- Representation of the plasma boundary typically used in stellarator optimization uses a non-unique poloidal angle.

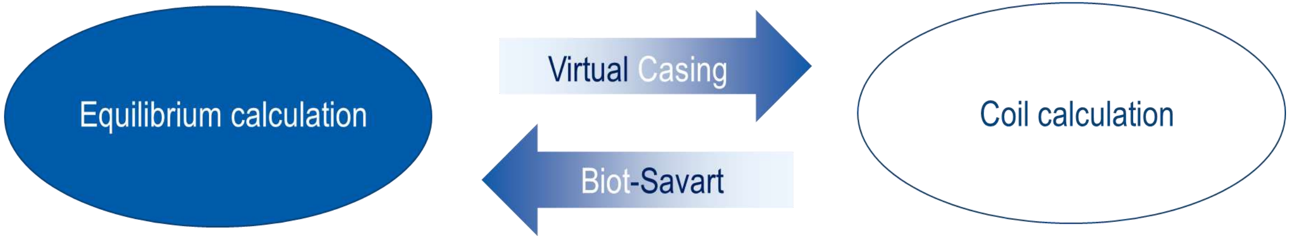
- This can cause an increase in the dimensionality of the search space and many additional minima can appear in the optimization landscape.

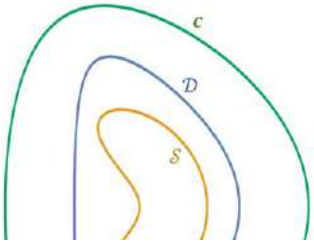
- This can be fixed by using a unique boundary representation.

- Our new, simple and intuitive boundary representation can improve the outcome of the optimization (in our cases typically by two orders of magnitude).



Combined plasma-coil optimization algorithms





i. Fixed-boundary optimization

Plasma boundary is the independent degree of freedom $\boldsymbol{z}$:

$$\boldsymbol{z} \equiv \mathcal{S}$$

ii. Generalized fixed-boundary optimization

Total normal magnetic field on computation boundary:

$\boldsymbol{z} \equiv B_{T,n}$ on $\mathcal{D}$ (which is fixed)

iii. Quasi-free-boundary optimization

Required external normal magnetic field on computational boundary:

$\boldsymbol{z} \equiv D_n$ on $\mathcal{D}$

iv. Free-boundary (coil) optimization

Coil geometry

$$\boldsymbol{z} \equiv \boldsymbol{c}$$

We categorized and analyzed four different combined plasma-coil (single stage) optimization approaches.

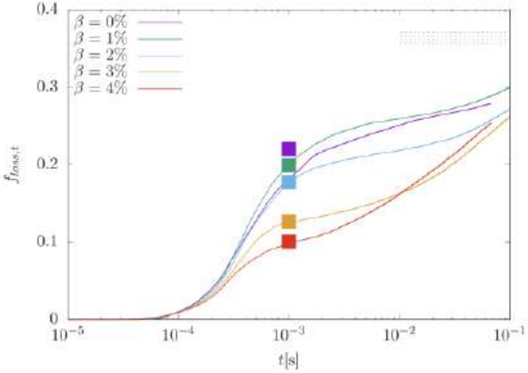
Since in general, $D_n \neq B_{E,n}$, we propose to target the quadratic-flux error in the optimization:

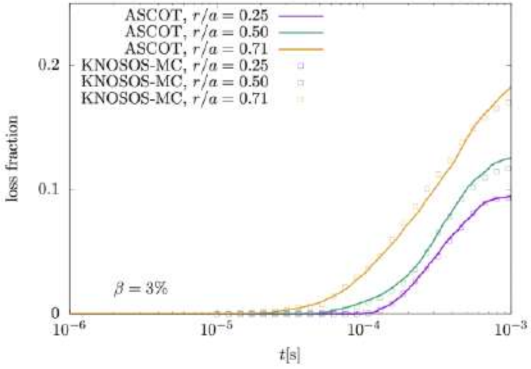
$$\boxed{\varphi_2 \equiv \int_{\mathcal{D}} \frac{1}{2}(D_n - \boldsymbol{B}_E \cdot \overline{\boldsymbol{n}})^2 \mathrm{d}\bar{s}}$$

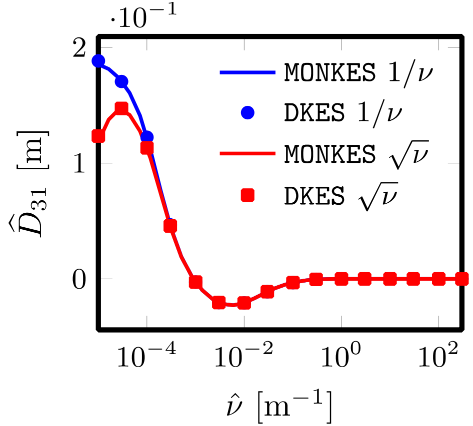
S.A. Henneberg, et al., JPP (2021)

New methods: fast and accurate neoclassical transport

Needed for the evaluation of neoclassical (NC) transport within the optimization loop:







- Γ_α (computed with KNOSOS): figure of merit for prompt losses of energetic ions (left).

J.L. Velasco, I. Calvo *et al.,* Nucl. Fusion 61, 116059 (2021).

- **KNOSOS-MC:** orbit-averaged accurate calculation of fast-ion transport in stellarators (center).

J.L. Velasco *et al.*, invited talk at ISHW (2022), I. Calvo *et al.*, invited talk at EFTC (2023).

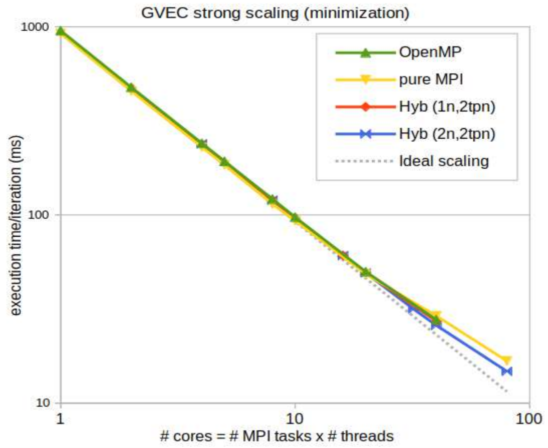
- **MONKES:** a fast (< minute/point) and accurate NC code for the evaluation of the bootstrap current (right).

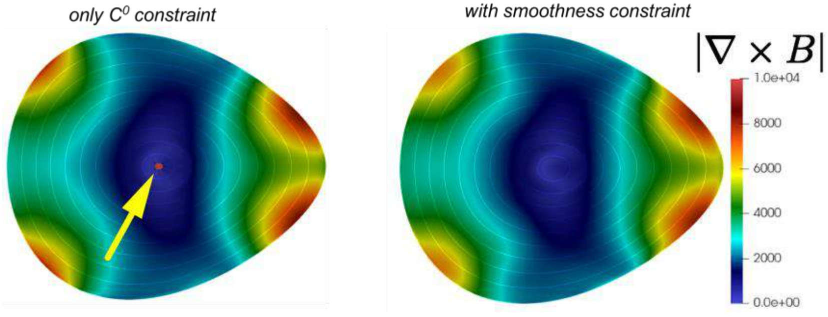
F. J. Escoto, J.L. Velasco, I. Calvo *et al.,* EFTC (2023).

GVEC progress

- Hybrid OpenMP+MPI parallelization by ACH-Garching:
  - Support of ACH-Garching key enabler for MPI parallelization of GVEC (needed ~15 PM) GVEC with OpenMP was limited to 1 node → Now hybrid OpenMP+MPI allows multiple nodes
  - 3D W7-X case with 80-P5 spline elements and (m,n)max=(10,10), run on cobra (MPCDF)→ Hybrid OpenMP+MPI most efficient, 1.8 speed-up from 1 → 2 nodes (each node with 2 MPI tasks×20 threads)
- New smoothness constraint at the magnetic axis: **Strong current spike at the axis** without the smoothness constraint,
  since asymptotic behavior $\sim \rho^m$ is not controlled
- Analysis of a new external vacuum solver for free-boundary GVEC
  - BIEST has been applied to Merkle's approach and tested against exact solution

  → Next step to couple GVEC with BIEST





Inventing fast metrics for alpha particle losses

- Novel fast guiding-center orbit classifiers testing for chaotic orbits were developed for the symplectic orbit tracer SIMPLE and successfully tested on various stellarator configurations.
- The novel topological classifier requires 30 times fewer orbit bounces than our earlier version, thereby pushing the speed-up of new metrics compared to traditional direct energetic particle loss computation to **> 1000**.
- Novel insights into the close analogy of resonant transport regimes in perturbed quasisymmetric stellarators and tokamaks.
- We foresee a major impact on optimized reactor designs.

Yellow: regular particles – can’t be lost

Green: chaotic trajectories

Blue: directly lost

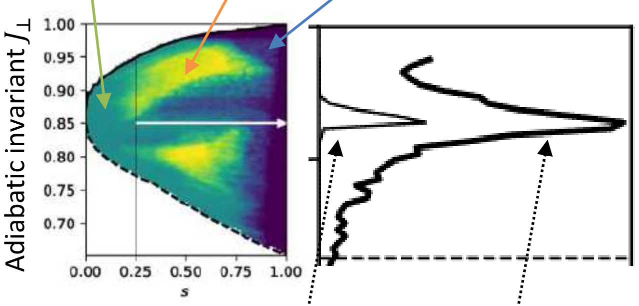


Fig. 1: Classification and lost energy fraction (collisionless and collisional)

C.G. Albert, et al., *JPP*, **89** 955890301, 2023

BOUT++ simulations for edge turbulence and transport

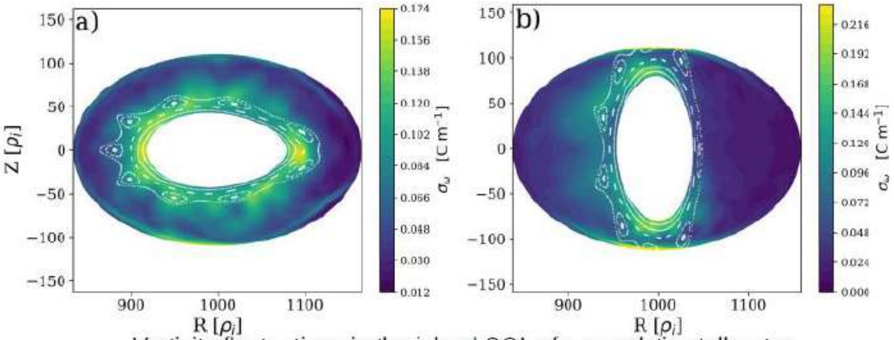
Fluid turbulence simulations have been performed in the edge of an analytic stellarator configuration with an island divertor [1]

- Fluctuations present throughout the scrape-off-layer
- Mean flows exhibit ballooning nature.

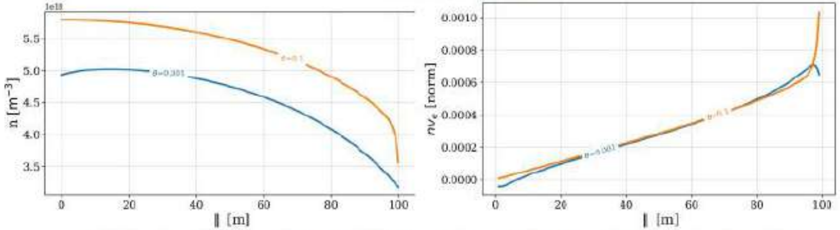
(Related work in TSVV-3: A.J. Coelho, et al., NF, 2022)

Hermes-3 [2], a multifluid model including atomic and neutral physics is being extended for stellarator applications

- The stellarator two-point model [3] has been implemented in Hermes-3
  - Fast 1D simulations for relevance to optimization
- Extension of 3D simulations to W7-X geometry ongoing



Vorticity fluctuations in the island SOL of an analytic stellarator configuration



Initial simulations of the stellarator 2-pt model in Hermes-3, showing the difference between tokamak and stellarator transport in the SOL.

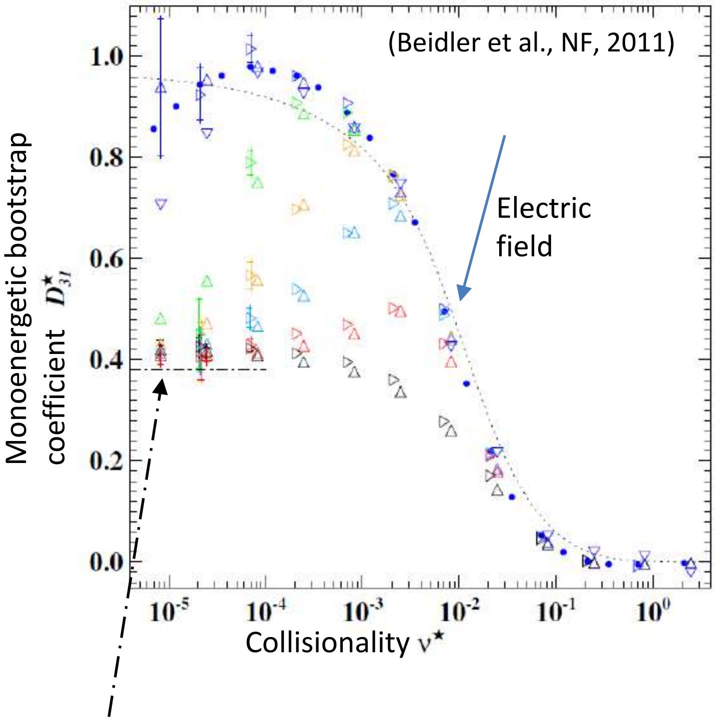
[1] B Shanahan et al., *NF Submitted* (2023)
[2] B Dudson et al., *Submitted* (2023)
[3] Y Feng et al., *PPCF* 53 024009 (2011)

Solving the bootstrap riddle at low collisionality

- Confirmed by several independent analytical derivations, the Shaing-Callen (SC) limit formula is *never reproduced by various drift kinetic equation (DKE) solvers* in the 1/v regime in real devices. In turn they show a trend of the bootstrap current to converge to the SC limit *in the presence of radial electric field.*

- Analytical and numerical examination of this paradox using the DKE solver NEO-2 showed that the off-set of bootstrap current from the SC limit is caused by high classes of locally trapped particles which can be detrapped directly to the passing region when traversing the local magnetic well. Such classes exist at any collisionality.

- The resulting offset diverges in the 1/v regime as $\nu^{-1/5}$ but converges in the presence of radial electric field as $\nu^{2/5}E_r^{-1/2}$. It is minimized in devices with low bounce averaged drift and in case of well-aligned local magnetic field maxima.



(Beidler et al., NF, 2011)

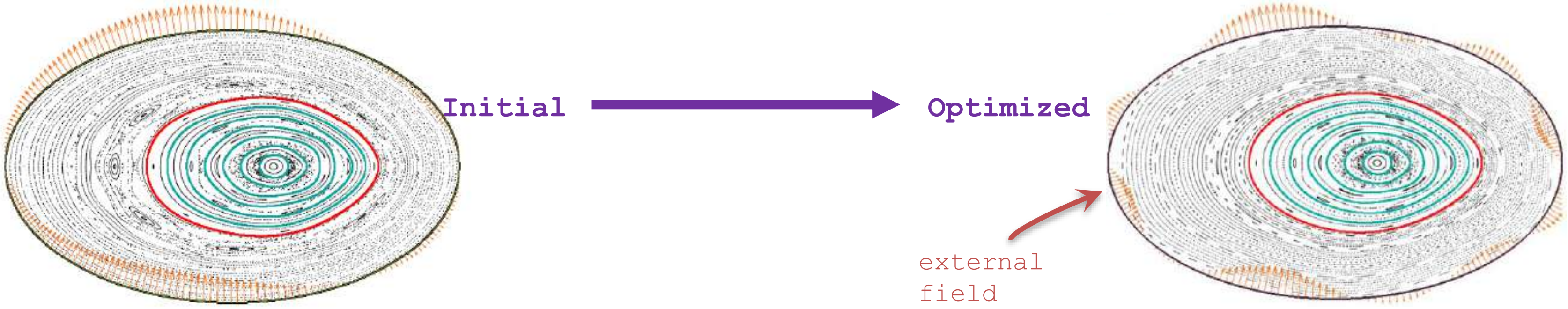
Electric field

Shaing-Callen result

Island healing & equilibrium β-limits

- Island healing at high-β achieved by combining free-boundary SPEC and SIMSOPT.

Baillod, Loizu, et al, PoP 2022



- New predictions of equilibrium β-limits in stellarators based on chaos-enhanced transport.

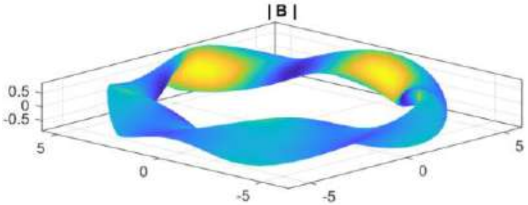
Baillod, Loizu, et al, accepted in JPP, 2023

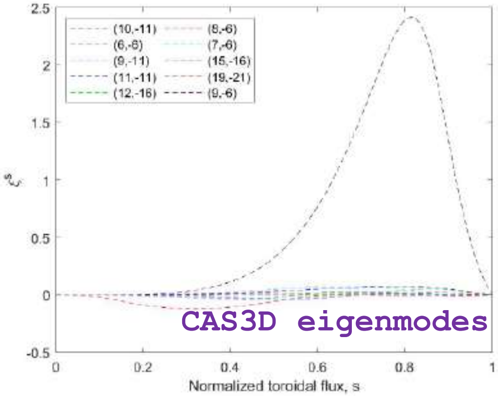
Beneficial for stellarator optimization: we may now tolerate a certain amount of islands/chaos when the corresponding increase in transport is anyway much smaller than the baseline turbulent transport.

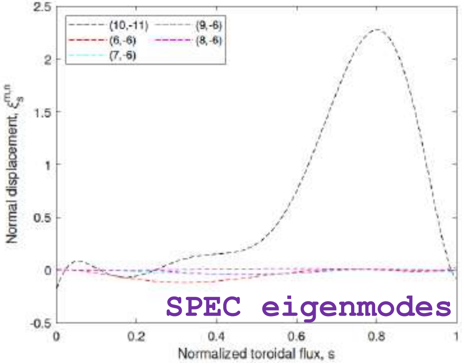
Stability studies

- Retrieved ideal stability in a stellarator with SPEC.

Kumar et al, PPCF, 2022







- Reproduced Glasser-Greene-Johnson tearing stability in a tokamak with SPEC.

Kumar, Loizu, et al, PPCF, 2023

- Reproduced nonlinear saturation of tearing modes with SPEC in a cylindrical tokamak

Loizu et al, accepted in JPP, 2023

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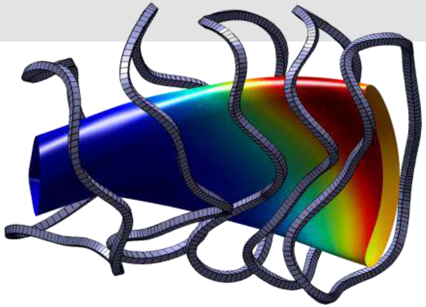
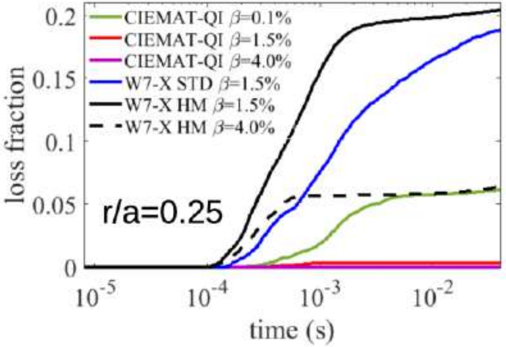
CIEMAT-QI

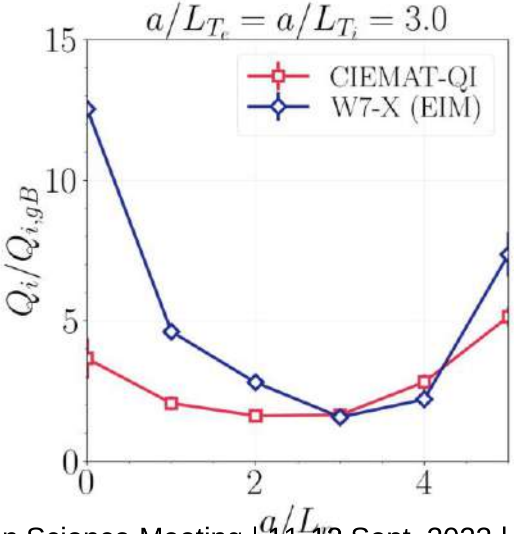
A quasi-isodynamic configuration



- 4 field periods
- ι profile avoiding low order rationals and compatible with island divertor.
- Ideal MHD stability.
- Low neoclassical transport.
- Reduced bootstrap current.
- **Very good confinement of fast ions at low β (~1.5%).**
- **Excellent confinement of fast ions at reactor-scale β (~4%)** (top right)**.**
- **Reduced turbulent transport** (bottom right)**.**
- **Preliminary set of filamentary coils** preserving the above properties.

E. Sánchez, J.L. Velasco, I. Calvo and S. Mulas, Nucl. Fusion 63, 066037 (2023).





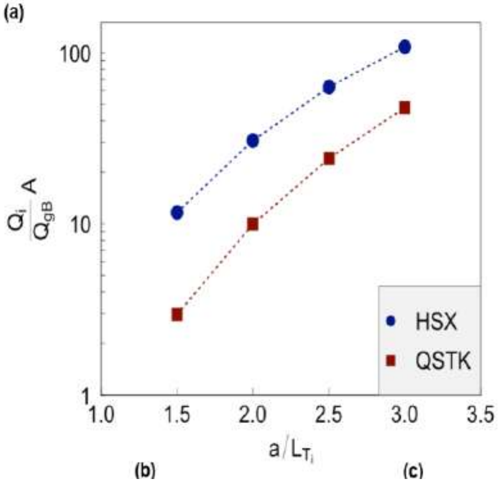
CIEMAT-QI belongs to the *family* of flat-mirror stellarators, which fulfil **maximum-*J* property at low β** and are thus resilient against error fields and plasma effects.

J. L. Velasco, I. Calvo, E. Sánchez, F.I. Parra, arXiv:2306.17506.

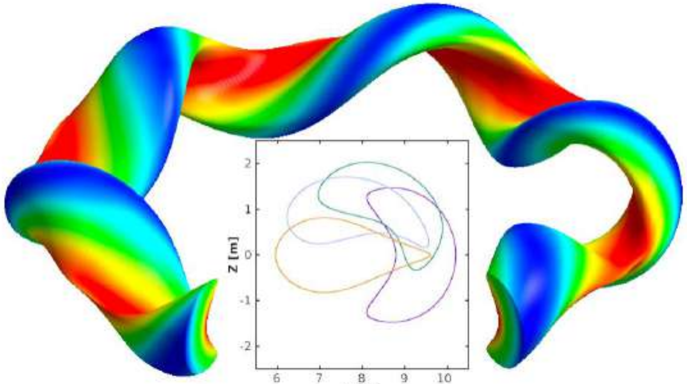
A stellarator with turbulence reduction

QSTK: a 6-periodic QH stellarator:

- Better fast-ion confinement than W7-X
- Lower thermal neoclassical transport than W7-X
- MHD stable
- ITG turbulence reduced



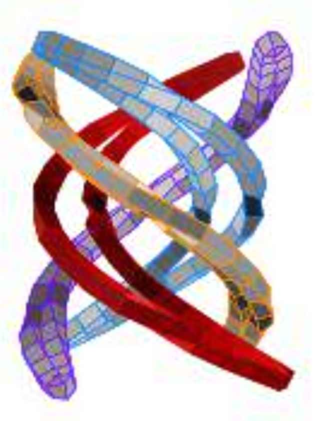
→ Efforts to combining turbulence reduction with precise QI (A.Goodman, G.Robert-Clark, P. Xanthopoulos)

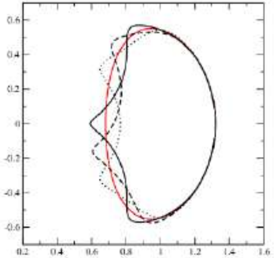


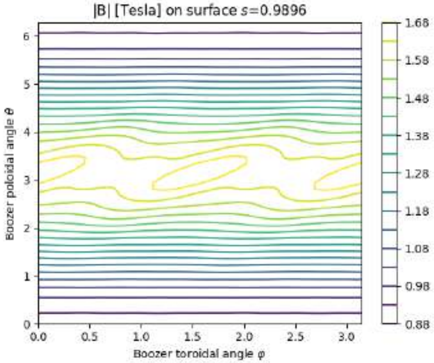
Roberg-Clark, et al., PRR (2023)

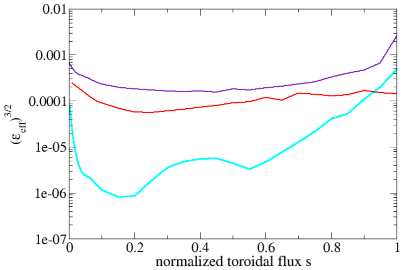
A compact stellarator-tokamak hybrid

- Can be operated as a tokamak or a stellarator or anything in between.
- Compact: aspect ratio down to 2.3
- Good QA accuracy (Smaller neoclassical transport than in W7-X)
- 4 simple saddle coils of a single type (in addition to TF coils + PF coils)
- Flux surfaces in vacuum with rotational transform of 0.3









S. Henneberg & G. Plunk, EUROfusion pinboard ID 35444, 36001

T. Schuett, S. Henneberg in preparation

Summary

Only selected results have been shown due to time restrictions, several topics were not mentioned (in depth) e.g.

- CAS3D built into ROSE,
- robust optimization via flat mirror magnetic fields,
- Introducing uncertainty quantification to 3D MHD equilibrium computation
- …

- New, improved or extended tools:
  - Unique boundary representation
  - Combined plasma-coil optimization algorithms
  - New codes to evaluate neoclassical transport quickly
  - Ideal MHD GVEC code development progress
  - New and fast metric for alpha-particle losses
  - 3D BOUT++ simulations for edge turbulence and transport
- Better understanding of stellarator physics:
  - Solving the bootstrap riddle
  - Island healing
  - New predictions of equilibrium β-limits in stellarators
  - Retrieved ideal stability in a stellarator with SPEC.
  - Reproduced Glasser-Greene-Johnson tearing stability in a tokamak with SPEC.
  - Reproduced nonlinear saturation of tearing modes with SPEC in a cylindrical tokamak
- Three new stellarator designs have been presented:
  - CIEMAT-QI
  - QSTK
  - Compact stellarator-tokamak hybrid

} Improved neoclassical confinement, turbulence transport, simpler coils

Ongoing and Future work

	Milestones promised until the end of this year:	Status
SD1.1	Integration of stella into stellarator optimization suites.	Achieved + work in progress
SD2.3	Accelerate computation of ASCOT on GPU hardware and via accelerated methods from SIMPLE and GORILLA.	Achieved + work in progress
SD2.4	Simulations of fast ion orbits in W7-X with experimentally relevant density and temperature profiles will be performed.	Achieved + work in progress
SD4.1	Development of a free-boundary version of GVEC	Partially
SD4.4	We will investigate analytically the advantages and disadvantages of different ways of representing the magnetic field with respect to reducing the stellarator optimization space and the ease of combining coil and stellarator optimization.	Achieved
SD6.2	A preliminary screening procedure of divertors can be automatized*.	Partially

*R. Davies, Y. Feng, S. A. Henneberg, paper in preparation

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SD6.2	A preliminary screening procedure of divertors can be automatized .	Partially
	Milestones promised until the end of next years:	**Status**
SD1.3	Integration of KNOSOS into stellarator optimization suite.	Partially
SD2.1	Develop numerical tools for the evaluation of the bootstrap current at low collisionality. This will allow to integrate them into stellarator optimization suite.	Achieved + work in progress

Ongoing and Future work

- Continue development, benchmark and validation of codes and integration in optimization suites.

- Improving existing designs, e.g.
  - CIEMAT QI – finding new configurations with different NFP (3,5,6)
  - combining QI & turbulence optimization, coil optimization, divertor designs
  - Investigating if the stellarator-tokamak-hybrid is a feasible approach

- Stellarator designs of the different topological classes will be investigated in detail and compared to each other with respect to different aspects, e.g.,
  - confinement,
  - stability,
  - heat exhaust options,
  - coil complexity

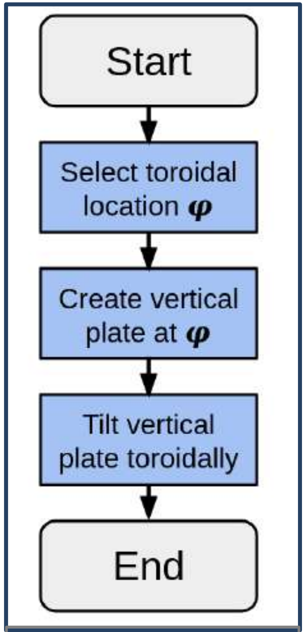
  with the new tools developed within this collaboration.

56 EUROfusion pinboard entries:
26 Journal publications
+ 30 conference contributions

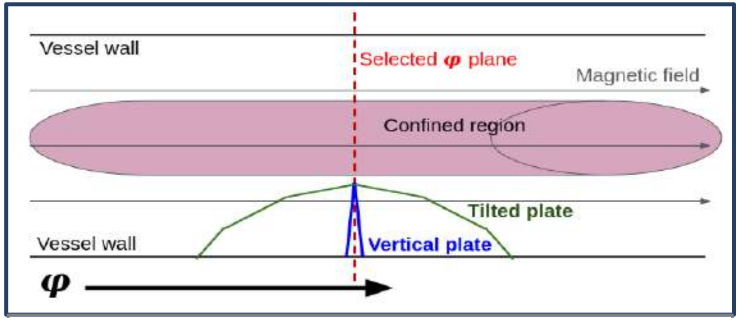
Year	Authors	Title	Journal	ID
	Henneberg, Plunk		PNAS	36001
	Henneberg, Plunk		NF	35444
	Velasco, et al.		NF	35385
	Loizu, Bonfiglio		JPP	35319
	Shanahan, Bold, Dudson		NFL	35241
2023	Roberg-Clark, et al.	Critical gradient turbulence optimization toward a compact stellarator reactor concept	PRR	33853
	Plunk, Helander		JPP	33573
	Goodman, et al.		JPP	33396
2023	Sanchez, et al.	A quasi-isodynamic configuration with good confinement of fast ions at low plasma beta	NF	33479
2023	Koerberl, et al.	Uncertainty quantification in three-dimensional magnetohydrodynamic equilibrium reconstruction via surrogate-assisted Bayesian inference	CPP	33310
2023	Mishchenko, et al.	Global gyrokinetic simulations of electromagnetic turbulence in stellarator plasmas	JPP	33186
	Baillod, et al.		JPP	33422
2022	d'Herbemont, et al.	Finite orbit width effects in large aspect ratio stellarators	JPP	31248
2022	Baillod, et al.	Stellarator optimization for nested magnetic surfaces at finite beta and toroidal current	PoP	31130
	Roberg-Clark, Xanthopolous, Plunk		JPP	33300
2022	Plunk, Helander	Energetic bounds on gyrokinetic instabilities. Part II. Modes of optimal growth	JPP	31388
2022	Roberg-Clark, Plunk, Xanthopolous	Coarse-grained gyrokinetics for the critical ion temperature gradient in stellarators	PRR	32012
2023	Albert, et al.	Alpha particle confinement metrics based on orbit classification	JPP	33398
2022	Albert,et al.	Resonant transport of fusion alpha particles in quasisymmetric stellarators	JPCS	32617
2022	Buchholz, et al.	Computation of neoclassical toroidal viscosity with the account of non-standard orbits in a tokamak	JPCS	31575
2022	Markl, et al.	Non-axisymmetric neoclassical transport from misalignment of equipotential and magnetic surfaces	PAST	33260
2022	Kumar, et al.	Nature of ideal MHD instabilities as described by multi-region relaxed MHD	PPCF	30819
2021	Henneberg, et al.	Combined Plasma-coils optimization	JPP	30211
2021	Henneberg, Helander, Drevlak	Representing the boundary of stellarator plasmas	JPP	29637
2021	Velasco, et al.	A model for the fast evaluation of prompt losses of energetic ions in stellarators	NF	29821
2021	Velasco, et al.	Fast simulations for large aspect ratio stellarators with the neoclassical code KNOSOS	NF	90820

Extra Slides

Divertor design: a "Tilted vertical plate" approach

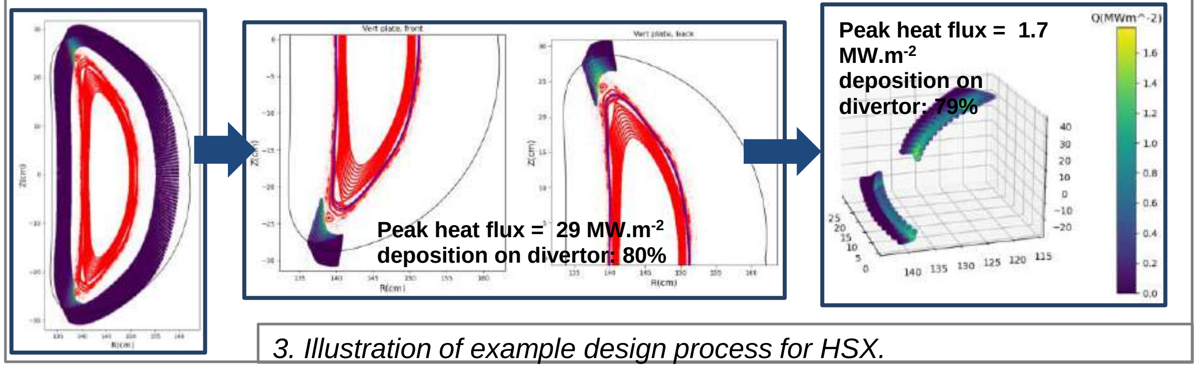


1. Divertor design flow chart



2. Cartoon of φ plane, vertical plate, tilted plate

- Current goal: Maximize wetted area / minimize heat loads
  - Heat load predictions made using EMC3-Lite
- An example design for HSX: most heat caught on divertor plates + small heat loads
- Future work:
  - Automation
  - Include engineering constraints
  - Optimize particle exhaust with simple models



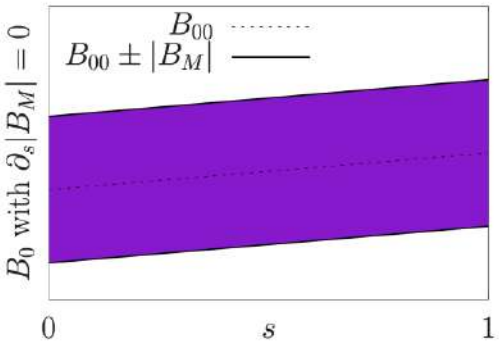
3. Illustration of example design process for HSX.

R. Davies, Y. Feng, S. A. Henneberg, paper in preparation

Strategy: robust optimization via flat mirror magnetic fields

Identified region of stellarator configuration space that fulfil **maximum-*J* property at low β**, which means reduced:

- Fast ion losses.
- Neoclassical transport of the bulk ions.
- Density-gradient-driven TEM turbulent energy transport.



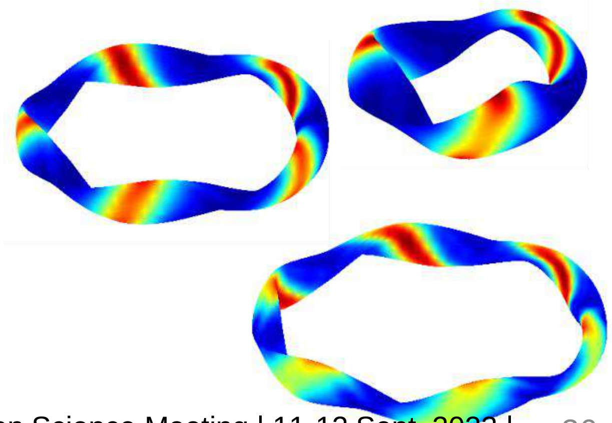
Flat mirror QI fields don’t need to be very close to exact omnigeneity and don’t require β or large $|E_r|$ **=> easier to design and to operate**

J. L. Velasco, I. Calvo, E. Sánchez, F.I. Parra, arXiv:2306.17506.

CIEMAT-QI belongs to this *family* of configurations.

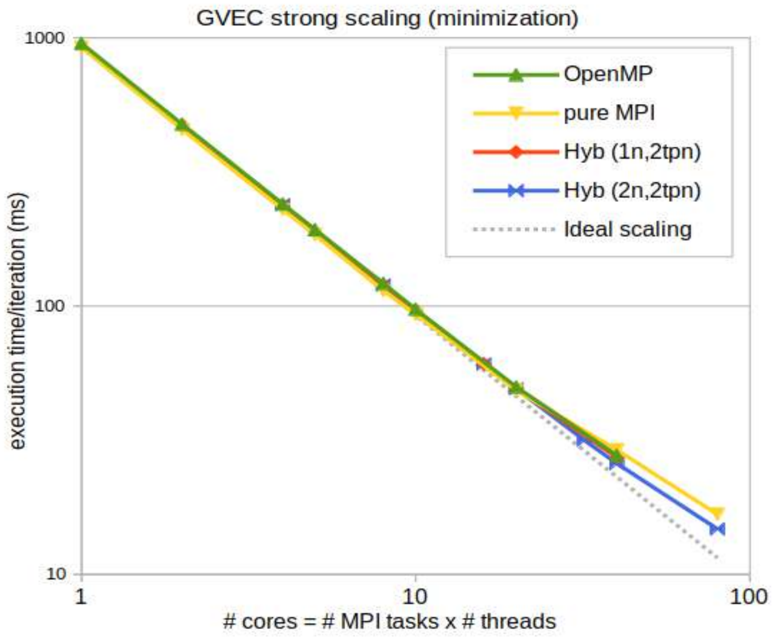
In parallel to CIEMAT-QI (N=4), <u>ongoing</u> optimisation for other periodicities

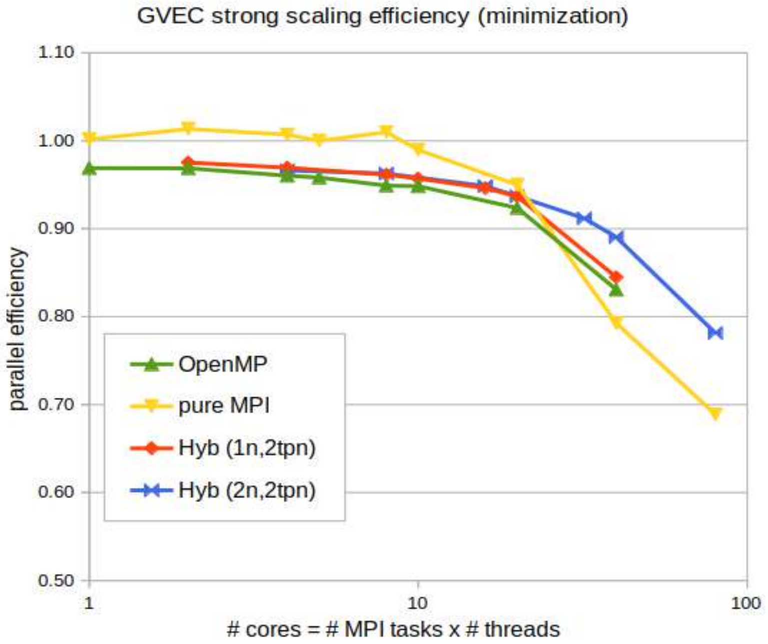
- Emphasis on balance between fast ion confinement, bootstrap current, aspect ratio and elongation.
- Promising results for 5 toroidal periods.



G. Godino-Sedano, *et al.*, contr. talk at Fusion HPC Workshop (2022), EFTC (2023).

GVEC: Hybrid OpenMP+MPI parallelization by ACH-Garching





- **Support of ACH-Garching key enabler** for MPI parallelization of GVEC (needed ~15 PM)
  GVEC with OpenMP was limited to 1 node ➔ **Now hybrid OpenMP+MPI allows multiple nodes**
- **3D W7-X case** with 80-P5 spline elements and $(m,n)_{max}$=(10,10), run on cobra (MPCDF)

➔ **Hybrid OpenMP+MPI most efficient, 1.8 speed-up from 1 → 2 nodes** (each node with 2 MPI tasks×20 threads)

GVEC: Analysis of a new external vacuum solver

- For free-boundary GVEC, the **external vacuum field** must be computed at the plasma boundary, including the effect of the plasma current $\mathcal{I}_p$
- Merkel [JCP1986] used in VMEC: $B = \underbrace{B_{\text{coil}} + B_{\mathcal{I}_p}}_{``B_0"} - \nabla\phi$

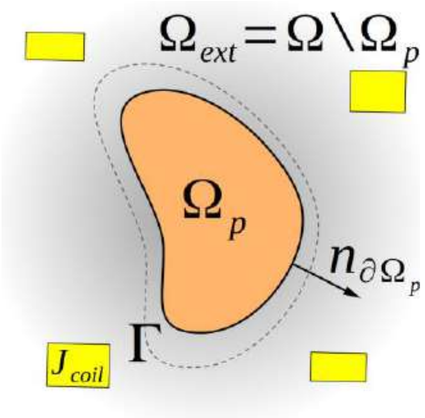
Arbitrariness in B_0

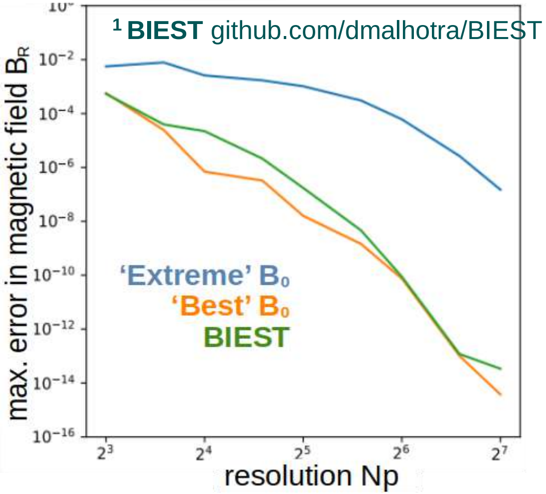
- Proven theoretically that B is **independent of B_0**
- But numerical accuracy depends on the model for B_0

Existing 3D boundary integral solver BIEST [1]

- applied to Merkel's approach
- tested against exact solution
- Accuracy comparable to the 'best' choice of B_0

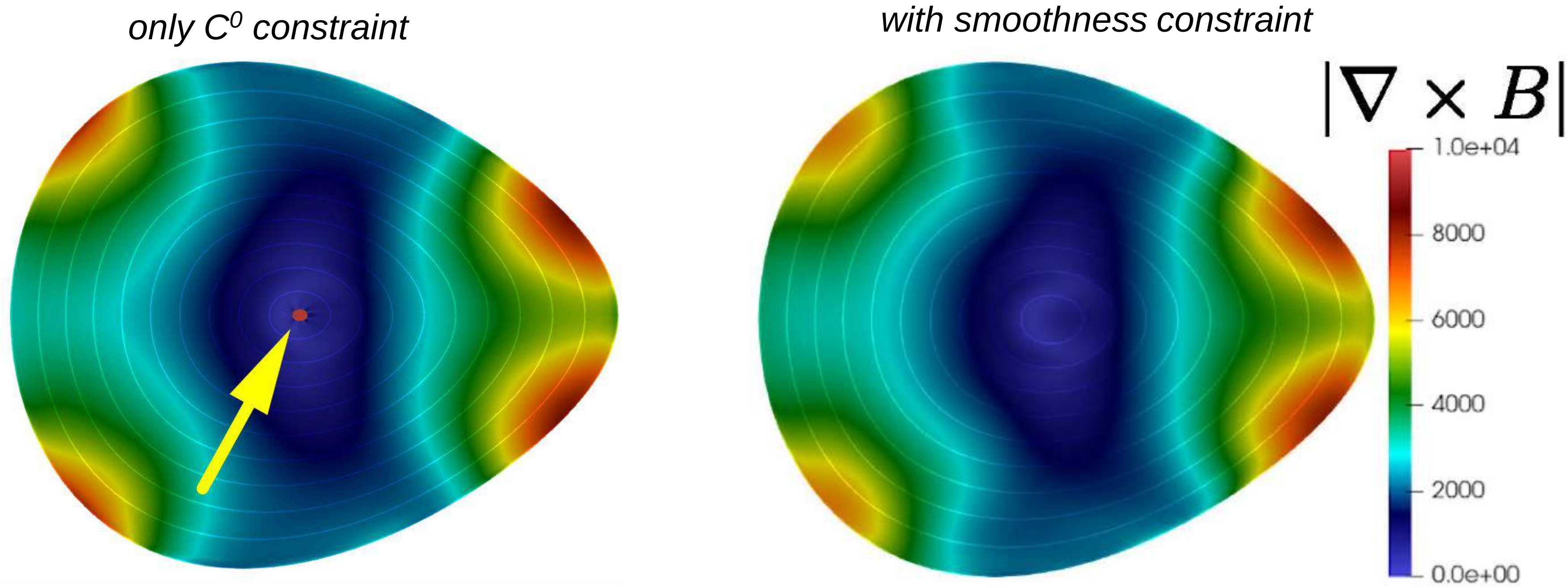
➔ **Next step is to couple GVEC**
+ BIEST for the external vacuum field + coil field evaluation





[1] **BIEST** github.com/dmalhotra/BIEST

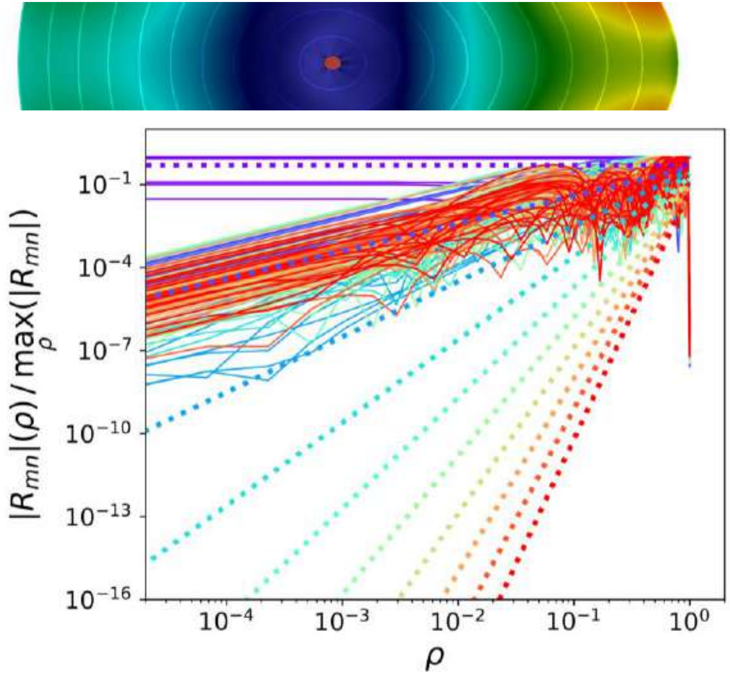
GVEC: New smoothness constraint at the magnetic axis



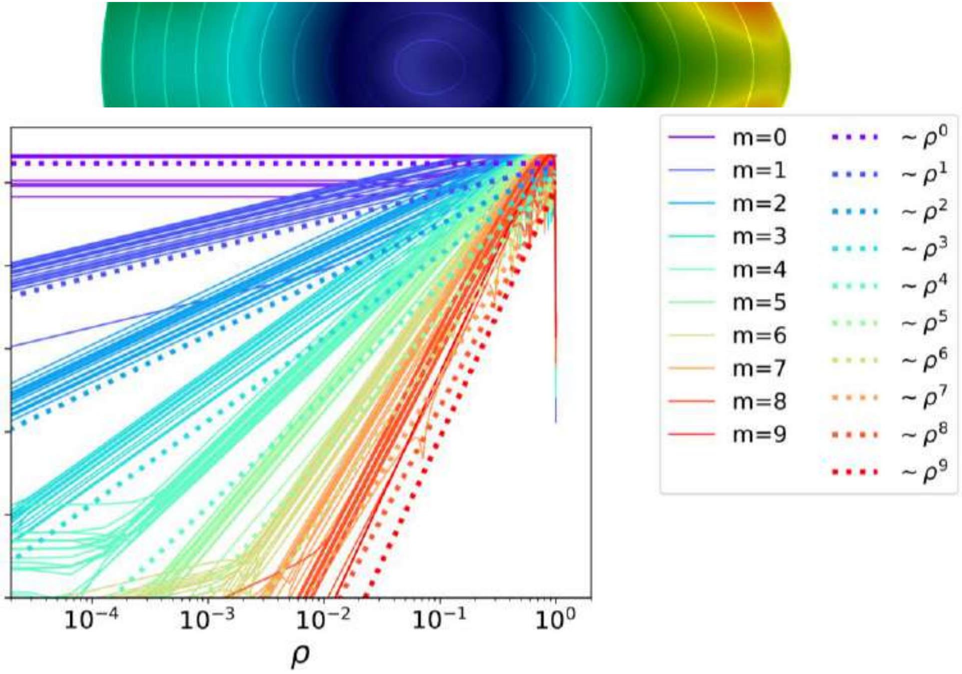
- **Strong current spike at the axis** without the smoothness constraint, since asymptotic behavior ~ ρ^m is not controlled

GVEC: New smoothness constraint at the magnetic axis

only C^0 constraint



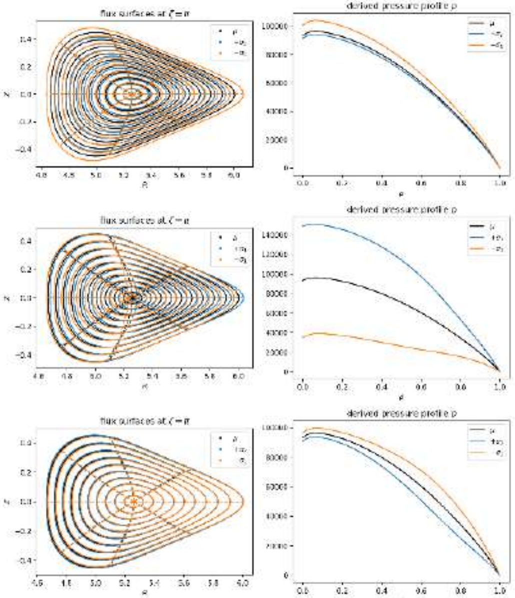
with smoothness constraint



➔ **All modes show correct asymptotic behavior $\sim\rho^m$** at magnetic axis with new smoothness constraint

3. Introducing uncertainty quantification to 3D MHD equilibrium computation

Fig. 3: Example of uncertainties in flux surface geometry and pressure profiles depending on number of principal components.

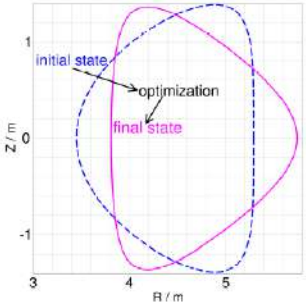


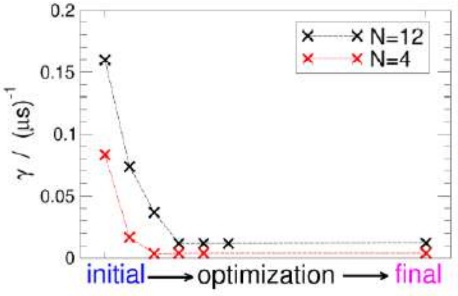
- Application of state-of-the-art data science methods of principal component analysis and polynomial chaos expansion to determine and store 3D MHD equilibria from the code VMEC together with uncertainties.
- Fast surrogates and dimensionality reduction allow efficient sampling in parameter spaces of equilibria.
- Application in both, stellarator optimization and equilibrium reconstruction (WP W7-X) in close cooperation with LHD/NIFS and the Simons collaboration on Hidden Symmetries and Fusion Energy.

Köberl R, von Toussaint U, Bungartz H-J, Schilling J, Albert C G and W7-X Team 2023 Uncertainty quantification in three-dimensional magnetohydrodynamic equilibrium reconstruction via surrogate-assisted Bayesian inference *Contributions to Plasma Physics* **63** e202200173

Linear global ideal MHD inside optimization loop (SD3.4)

example 1:
tokamak triangularity





- ROSE: configuration optimization
  CAS3D: linear global ideal MHD stability
- reduce resource requirements of global MHD stability target by use of symmetry properties of configuration
- effective reduction of growth rates irrespective of targeted toroidal node number (tokamak) or mode family and mode number size (stellarator)
- example 1: with the profiles chosen, positive triangularity is necessary for linear ideal MHD stability
- example 2: optimization reveals interrelations between configuration properties, e.g. simultaneous increase of magnetic-field mirror and Γ_c for

example 2: stellarator stability
6-period quasi-helical configuration