Comparison of the DESC and VMEC 3D Equilibrium Codes

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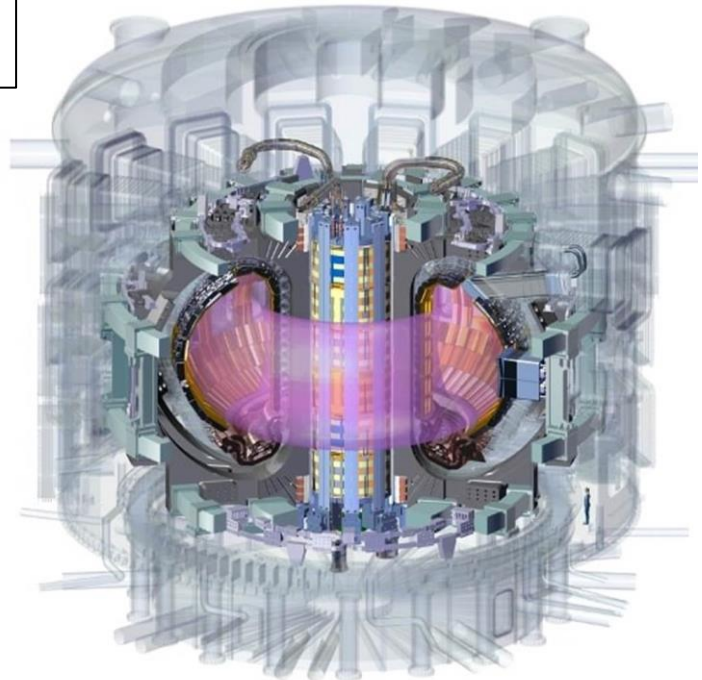
Outline

- Motivation
- DESC and VMEC Code Description
- Comparison Methods
- Comparison Results
- Summary + Future Work

Plasma Equilibria: What and Why?

<u>Plasma Equilibrium</u>: Configuration of magnetic fields that describes a plasma in **steady-state**

- Reactor Design and Optimization
- Experimental Reconstruction
- Necessary for many further plasma physics studies
  - Particle Transport
  - Stability



https://www.ansys.com/news-center/press-releases/ansys-enables-iter-organization-design-worlds-largest-highly-sustainable-nuclear-fusion-power-plant

Stellarator Optimization - VMEC

$$\frac{\partial X_j^{mn}}{\partial t} = F_j^{mn}$$

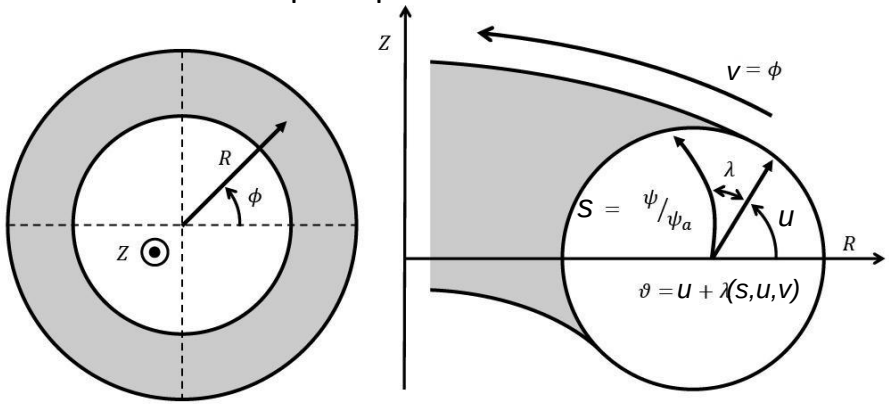
$$W = \int_V \left(\frac{B^2}{2\mu_0} + \frac{p}{\gamma - 1} dV \right)$$

- Spectral inverse equilibrium code (Hirshman and Whitman, 1983)
  - Solves 'inverse' equilibrium problem
  - want location of flux surfaces R,Z as function of computational domain (**s**,**u**,**v**)
- Assumes Nested Flux Surfaces, Ideal MHD
- Fourier series on flux surfaces, defined only on discrete radial grid
- Angular derivatives analytic, but radial derivatives are finite difference
- Minimizes energy with steepest-descent method based on variational principle

$$R(s,u,v) = \sum_{m=0,n=-N}^{M,N} R_{mn,c}(s)cos(mu - nvN_{FP}) + R_{mn,s}(s)sin(mu - nvN_{FP})$$

$$\lambda(s,u,v) = \sum_{m=0,n=-N}^{M,N} \lambda_{mn,c}(s)cos(mu - nvN_{FP}) + \lambda_{mn,s}(s)sin(mu - nvN_{FP})$$

$$Z(s,u,v) = \sum_{m=0,n=-N}^{M,N} Z_{mn,c}(s)cos(mu - nvN_{FP}) + Z_{mn,s}(s)sin(mu - nvN_{FP})$$



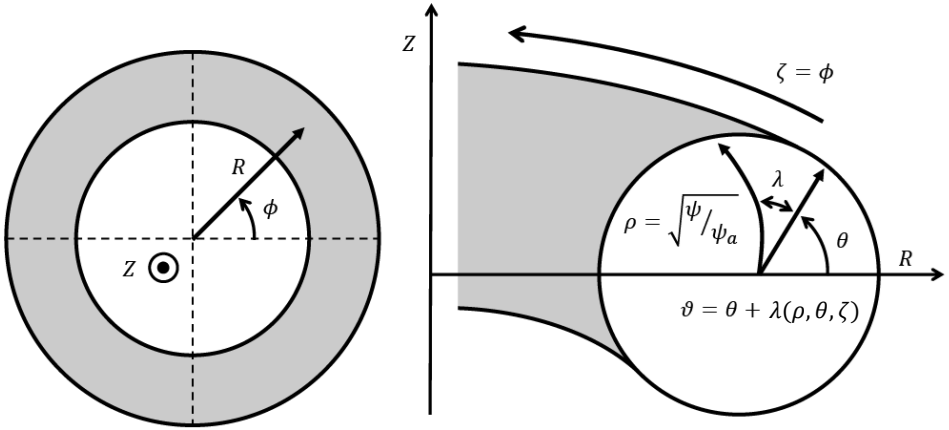
Stellarator Optimization - DESC

- 3D Ideal MHD Equilibrium Code
- Assumes Nested Flux Surfaces
- Inverse Equilibrium Problem
- **Minimizes Force Error Directly**
- **Pseudospectral Code**

$$\boldsymbol{F} = \boldsymbol{J} \times \boldsymbol{B} - \nabla p = 0$$

(Dudt and Kolemen 2020)

3D Spectral Representation of $\mathbf{x} = (R, \lambda, Z)$ using Fourier-Zernike Basis



Force Error as an Error Metric

$$\boldsymbol{F} = \boldsymbol{J} \times \boldsymbol{B} - \nabla p = 0$$

- Goal is to satisfy MHD equilibrium force balance in volume
- Looking at residual force error is an **intuitive** metric of how well the governing equations are being solved
- Use force error residual as metric to compare DESC and VMEC codes
- VMEC does not output force error
  - -> Must calculate from outputs (R,Z,λ)

Force Error is Calculated from VMEC Starting with R,Z,λ

- Read in Fourier coefficients from VMEC wout file
  - convert λ from half -> full mesh
- Find necessary angular derivatives **analytically**
- Find necessary radial derivatives **numerically**
  - finite difference, splines, etc.
- Multiply out in real space to find force error **F**
- Use **F** to define error metrics

$$\boxed{R(s,u,v), Z(s,u,v), \lambda(s,u,v)}$$

$$\mathbf{e}_s = \begin{bmatrix} \partial_s R \\ 0 \\ \partial_s Z \end{bmatrix} \qquad \mathbf{e}_u = \begin{bmatrix} \partial_u R \\ 0 \\ \partial_u Z \end{bmatrix} \qquad \mathbf{e}_v = \begin{bmatrix} \partial_v R \\ R \\ \partial_v Z \end{bmatrix}$$

$$\sqrt{g} = \mathbf{e}_s \cdot \mathbf{e}_u \times \mathbf{e}_v$$

$$B^u = \frac{1}{\sqrt{g}}\left(\chi' - \psi' \frac{\partial \lambda}{\partial v}\right) \qquad B^v = \frac{1}{\sqrt{g}}\psi'\left(1 + \frac{\partial \lambda}{\partial u}\right)$$

$$J^s = \frac{1}{\mu_0 \sqrt{g}}\left(\frac{\partial B_v}{\partial u} - \frac{\partial B_u}{\partial v}\right)$$

$$J^u = \frac{1}{\mu_0 \sqrt{g}}\left(\frac{\partial B_s}{\partial v} - \frac{\partial B_v}{\partial s}\right)$$

$$J^v = \frac{1}{\mu_0 \sqrt{g}}\left(\frac{\partial B_u}{\partial s} - \frac{\partial B_s}{\partial u}\right)$$

$$\boxed{\boldsymbol{B}(s,u,v), \boldsymbol{J}(s,u,v)}$$

$$F_s = \sqrt{g}(J^v B^u - J^u B^v) + p'$$

$$F_\beta = J^s$$

$$\boxed{\boldsymbol{F}(s,u,v)}$$

Force Error Metrics

$$\boldsymbol{F} = \boldsymbol{J} \times \boldsymbol{B} - \nabla p = 0$$

- **Volume-Averaged Force Error**
  - Taken from $s = 0.1 \rightarrow s = 0.99$

$$< F >_{vol} = \frac{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \int_{s=0.1}^{0.99} |F||\sqrt{g}| ds d\phi d\theta}{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \int_{s=0.1}^{0.99} |\sqrt{g}| ds d\phi d\theta}$$

- **Flux-Surface-Averaged Force Error**

$$< F >_{fsa} (s) = \frac{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} |F(s)||\sqrt{g}(s)| d\phi d\theta}{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} |\sqrt{g}(s)| d\phi d\theta}$$

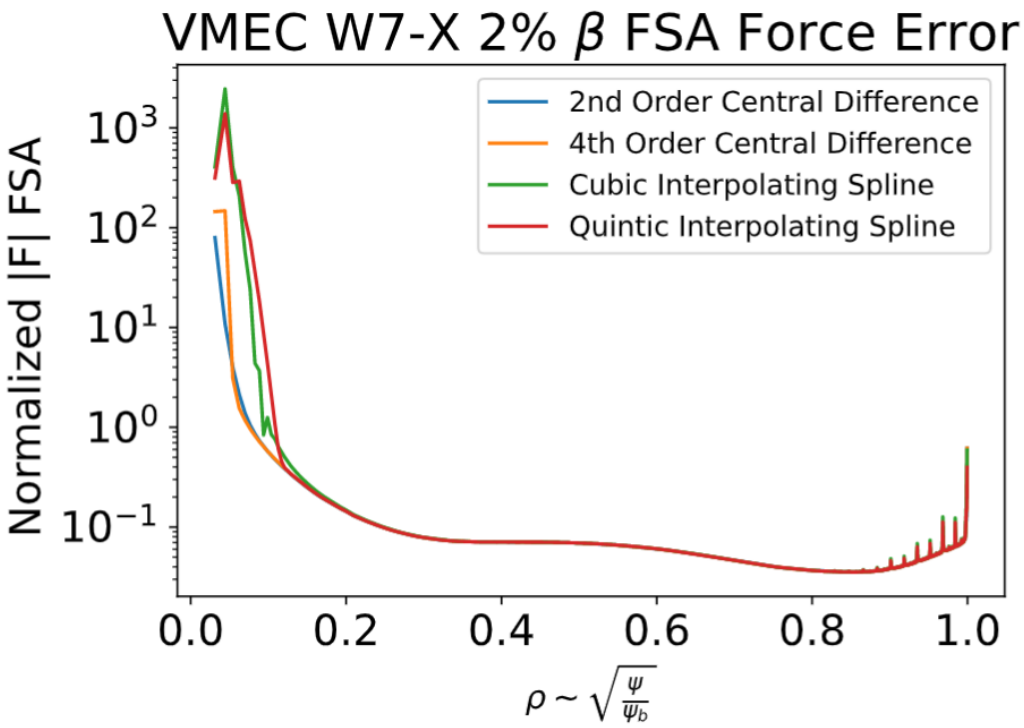
- **Both normalized by pressure gradient volume average**

$$< |\nabla p| >_{vol} = \frac{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \int_{s=0}^{1} |\nabla p||\sqrt{g}| ds d\phi d\theta}{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \int_{s=0}^{1} |\sqrt{g}| ds d\phi d\theta}$$

Calculated Force Error Insensitive to Radial Derivative Method

Only near-axis changes significantly with method

2nd Order Central Differences used for remainder of results shown in this presentation

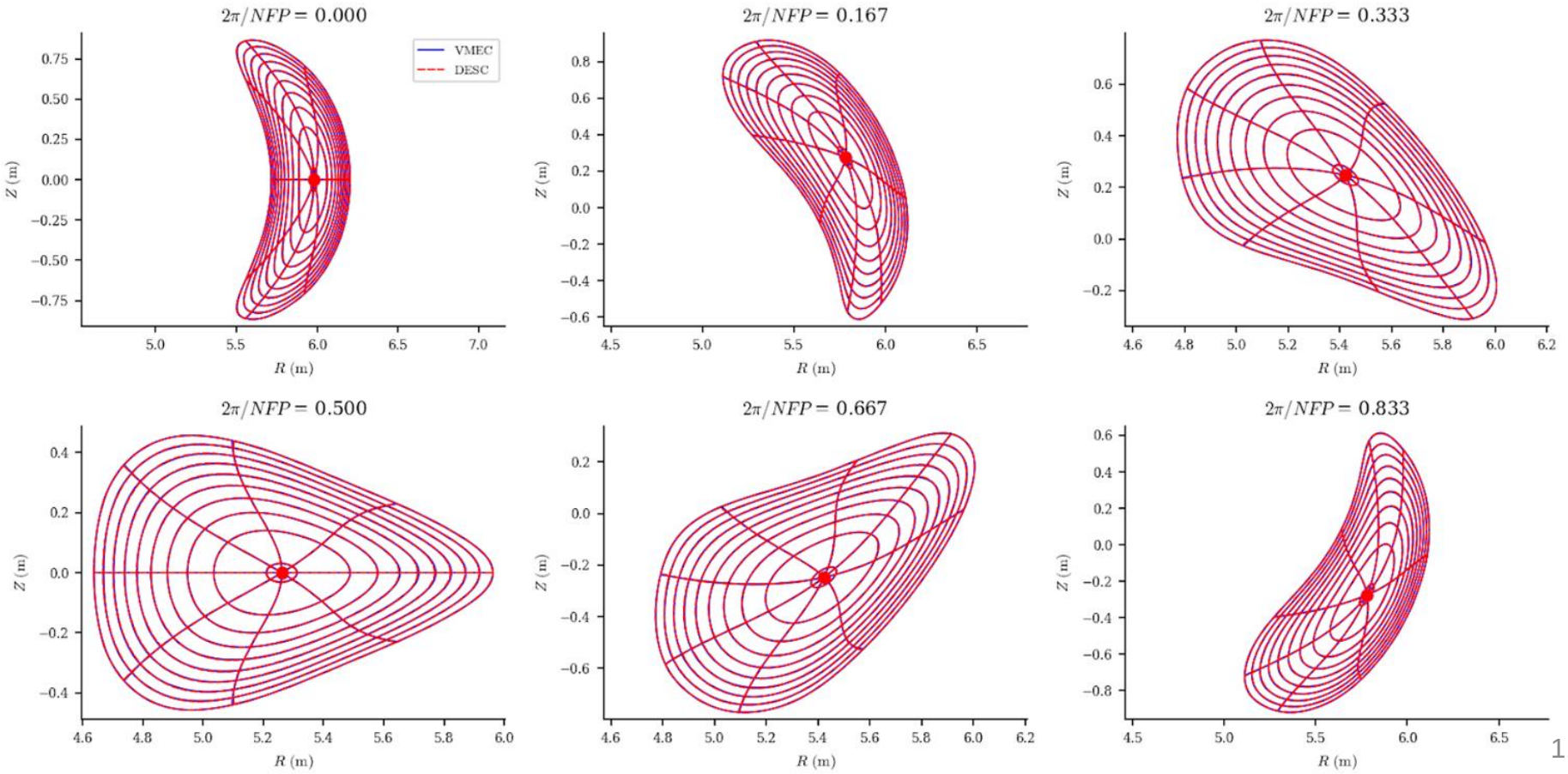


Code Solution Comparison Procedure

- The same W7X-like input boundary and profiles (available on DESC github) were used for all comparisons
- Angular and radial resolutions for each code was varied and ran to form a set of solutions
- Normalized force balance error metrics for each solution was calculated
- All solutions were ran in **fixed boundary** mode
- All solutions were ran on **identical architectures**
  - A single AMD EPYC 7281 CPU core with 32GB of RAM on PPPL's portal computing clusters

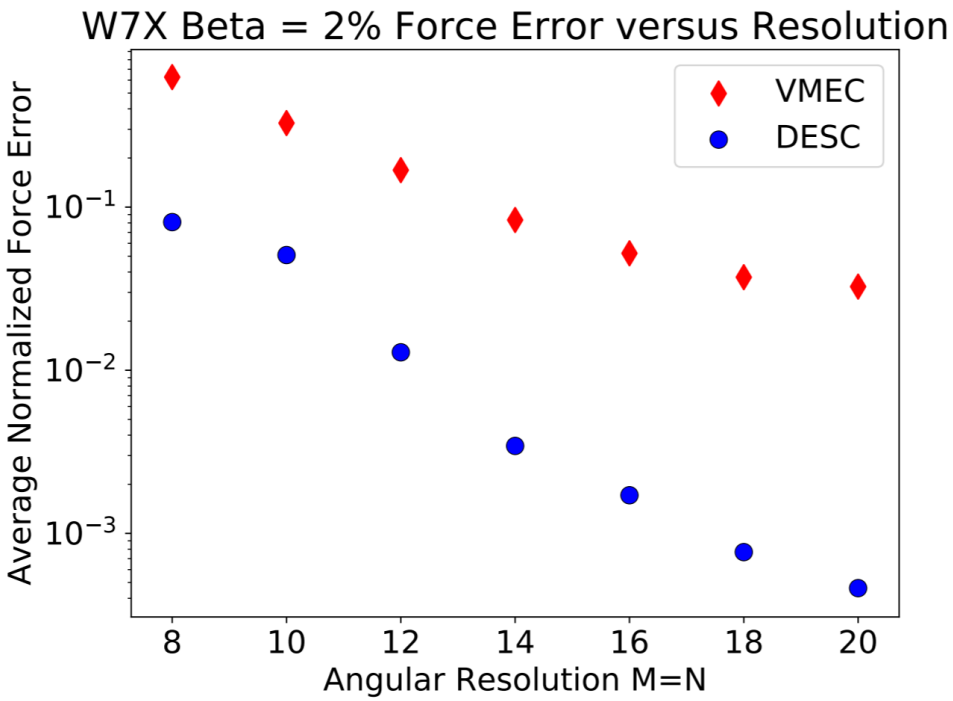
	Angular Resolution	**Radial Resolution**	**Other Parameters**
DESC	M=N=[8,10,12,14,16,18,20]	L=M=N	Fringe and ANSI spectral indexing
VMEC	M=N=[8,10,12,14,16,18,20]	NS=[256,512,1024]	FTOL=[1E-4,1E-8,1E-12]

Solution Comparison - Flux Surfaces Indistinguishable by Eye



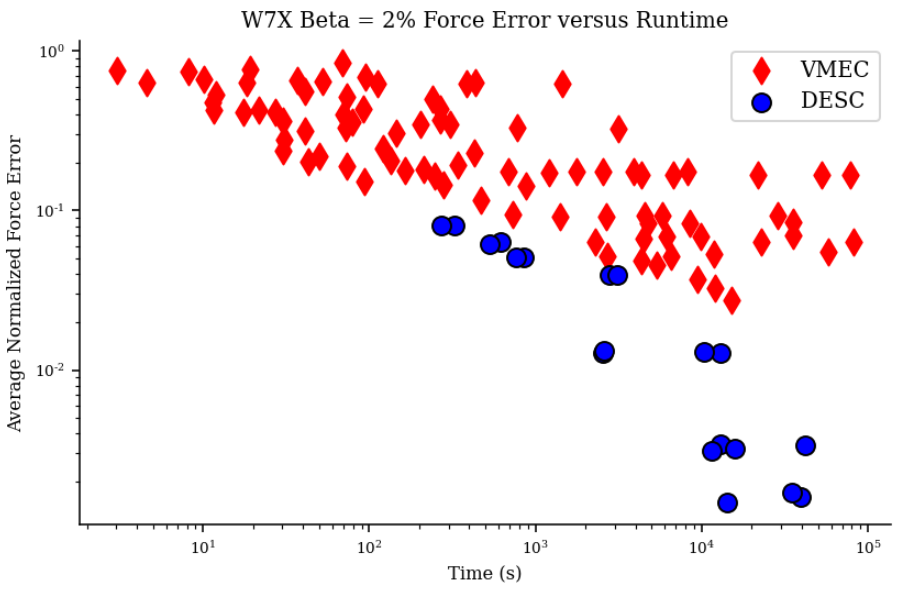
For Given Resolution, DESC has lower Force Error

W7X M=N=12			
	Energy (J)	$\lvert \mathbf{F} \rvert / \lvert \nabla p \rvert$	Runtime (1 CPU)
DESC (L=12)	8.4648759e+07	0.013	0.71 hours
VMEC (ns=1024)	8.4648752e+07	0.168	1.19 hours



For Given Time to Solution, DESC has lower Force Error

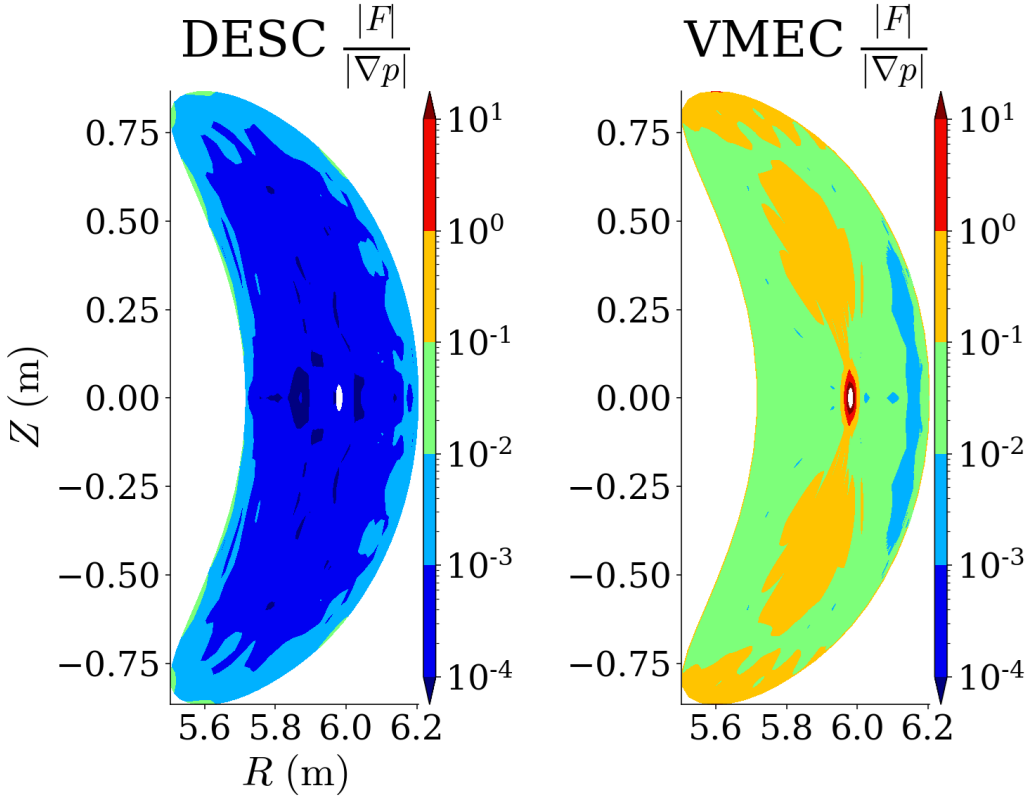
W7X M=N=12			
	Energy (J)	**|F|/|∇p|**	Runtime (1 CPU)
DESC (L=12)	8.4648759e+07	0.013	0.71 hours
VMEC (ns=1024)	8.4648752e+07	0.168	1.19 hours



$$< F >_{vol} = \frac{\int_{\theta=0}^{2\pi}\int_{\phi=0}^{2\pi}\int_{\rho=0.1}^{0.99} |F||\sqrt{g}| d\rho d\phi d\theta}{\int_{\theta=0}^{2\pi}\int_{\phi=0}^{2\pi}\int_{\rho=0.1}^{0.99} |\sqrt{g}| d\rho d\phi d\theta}$$

VMEC Force Error is Noticeably Higher Near-axis

- This could be due to VMEC's Fourier coefficients not explicitly obeying analyticity constraint near axis



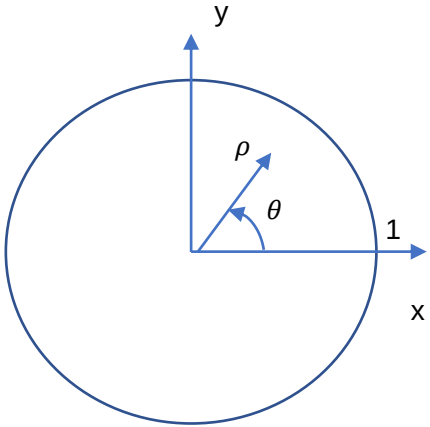
[1](Lewis and Bellan, 1990)

Analyticity Constraints for Functions in Polar Domains

If a function $f(\rho,\theta)$ is analytic everywhere on the unit disk, then

$$\lim_{\rho\to 0}\frac{a_m}{\rho^m} < \infty \qquad \lim_{\rho\to 0}\frac{b_m}{\rho^m} < \infty$$

i.e $a_m, b_m \sim \rho^m$ as $\rho \to 0$



where

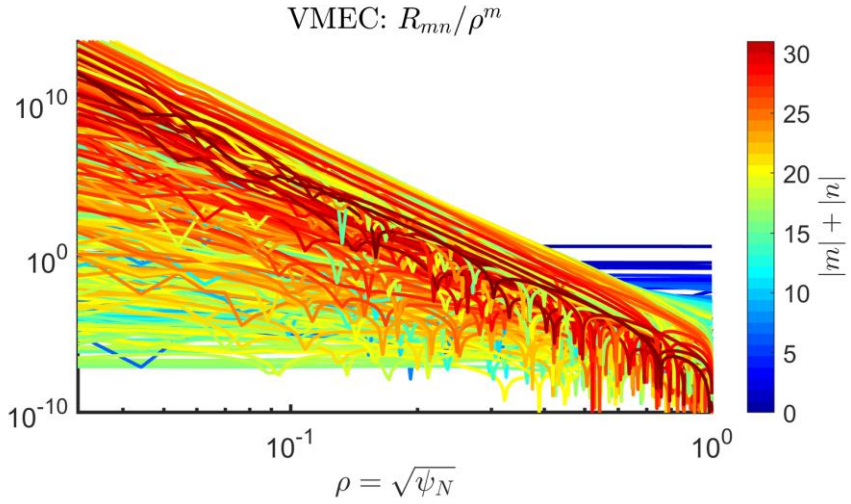
$$f(\rho,\theta) = \sum_{m=0}^{\infty} a_m(\rho)\cos(m\theta) + \sum_{m=0}^{\infty} b_m(\rho)\,sin(m\theta)$$

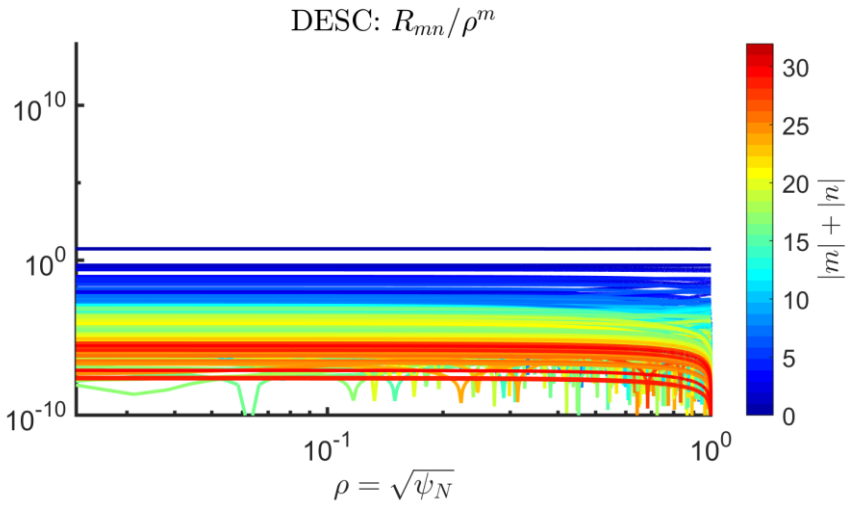
We expect any **physical quantity** (like the magnetic field), to be **analytic**

The Zernike basis radial-poloidal mode coupling **automatically satisfies this constraint**

Analytic Constraint Near Axis

- Fourier coefficients of an analytic function must scale as ρ^m near axis (Lewis and Bellan 1990)
- DESC coefficients obey this inherently due to Zernike basis, VMEC do not, especially for higher order modes



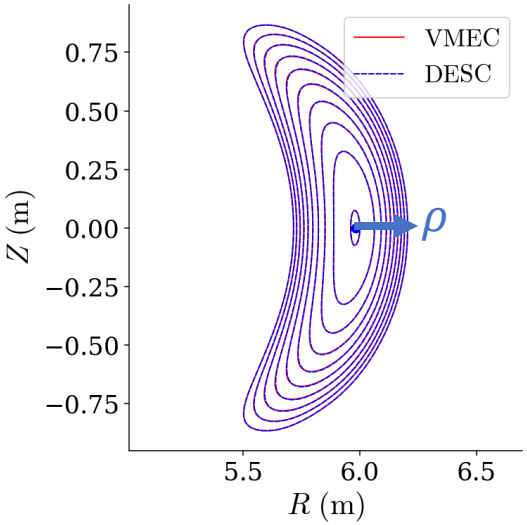


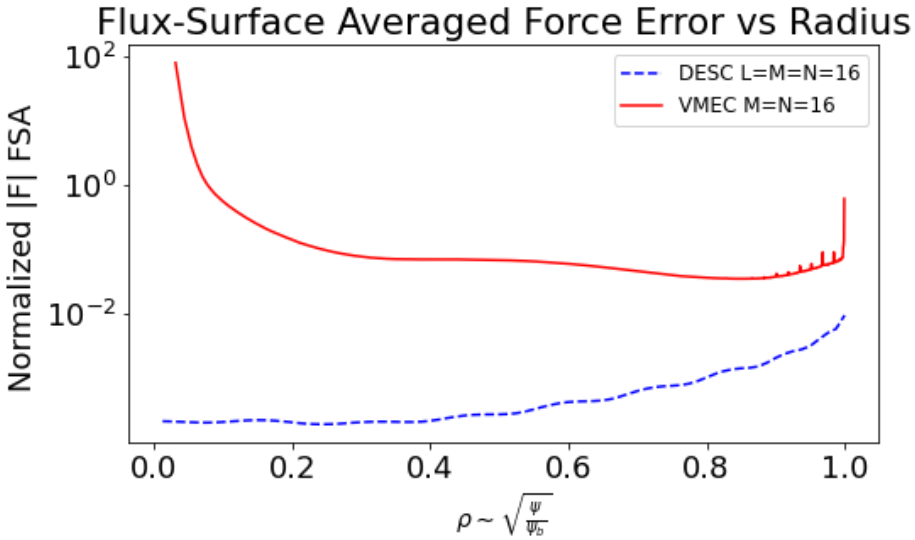
Plots Courtesy of Daniel Dudt

DESC compares well to VMEC – Force Error

Surface-Averaged Force Balance Error **lower in DESC** than VMEC

VMEC error spikes near $\rho \to 0$: Issues at axis!



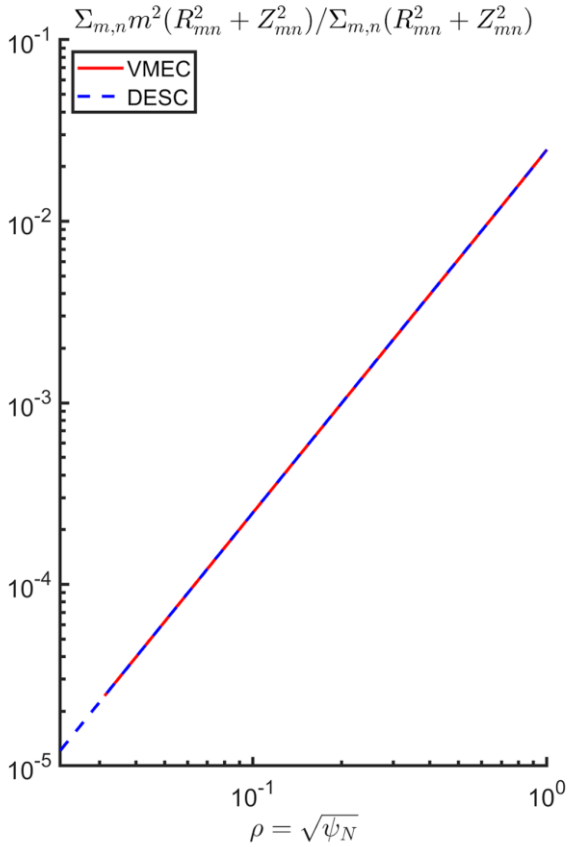


Both DESC and VMEC Poloidal Angle are Optimal

- Spectral condensation as defined by Hirshman and Meier (1985)

$$M(p,q) \equiv \frac{\Sigma_{m=1}\, m^q S_p(m)}{\Sigma_{m=1} S_p(m)}$$

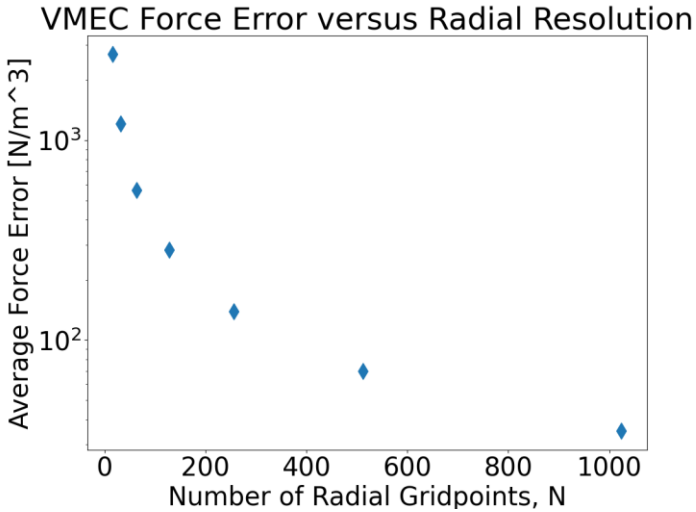
- Minimization of M wrt poloidal angle corresponds to an optimally condensed Fourier spectrum -> explicit constraint in VMEC
- DESC poloidal angle found through optimization is as optimal as VMEC's

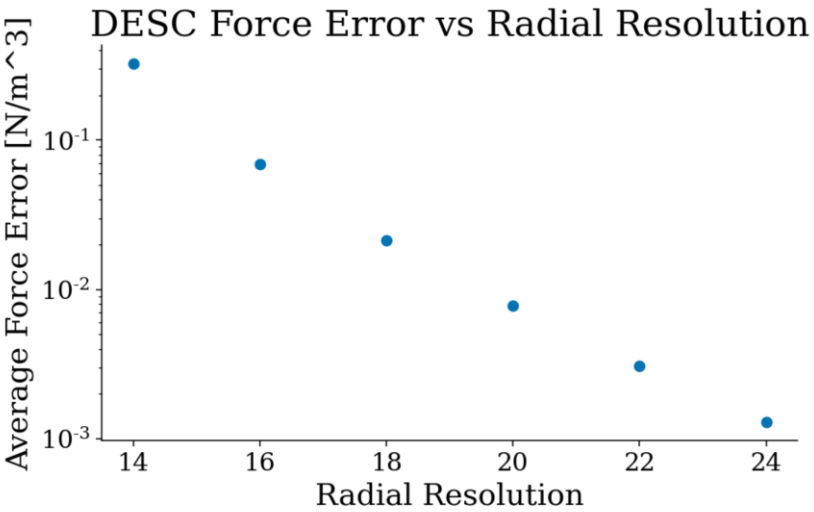


Plot Courtesy of Daniel Dudt

DESC compares well to VMEC – Convergence (DSHAPE)

	Angular Convergence	Radial Convergence
DESC	Exponential	**Exponential**
VMEC	Exponential	**Algebraic** $\boldsymbol{O}\left(N_{radial}^{-1}\right)$





Conclusions

- DESC **more accurate** than VMEC at given resolution or time-to-solution
- DESC solution accuracy better than VMEC **near axis**
- DESC radial convergence **not limited by finite differences**
- Both DESC and VMEC find similarly optimal poloidal angle
- Future work can make DESC faster – pre-compilation of objective, parallelize across CPUs/GPUs

Thanks! Questions?

Check out our Code!

Publication: Dudt et. al. *Phys. Plasmas*. 2020.

Repository: https://github.com/PlasmaControl/DESC

Python Package: `pip install desc-opt`

Backup

What DESC Solves

Inputs: $\mathrm{R_b}(\theta,\zeta), \mathrm{Z_b}(\theta,\zeta), p(\rho), \iota(\rho)$

$$\mathbf{e}_\rho = \begin{bmatrix} \partial_\rho R \\ 0 \\ \partial_\rho Z \end{bmatrix} \qquad \sqrt{g} = \mathbf{e}_\rho \cdot \mathbf{e}_\theta \times \mathbf{e}_\zeta$$

$$\mathbf{e}_\theta = \begin{bmatrix} \partial_\theta R \\ 0 \\ \partial_\theta Z \end{bmatrix} \qquad B^\theta = \frac{\psi'}{\sqrt{g}}\left(\iota - \frac{\partial \lambda}{\partial \zeta}\right)$$

$$\mathbf{e}_\zeta = \begin{bmatrix} \partial_\zeta R \\ R \\ \partial_\zeta Z \end{bmatrix} \qquad B^\zeta = \frac{1}{\sqrt{g}}\psi'\left(1 + \frac{\partial \lambda}{\partial \theta}\right)$$

$$J^\rho = \frac{1}{\mu_0\sqrt{g}}\left(\frac{\partial B_\zeta}{\partial \theta} - \frac{\partial B_\theta}{\partial \zeta}\right)$$

$$J^\theta = \frac{1}{\mu_0\sqrt{g}}\left(\frac{\partial B_\rho}{\partial \zeta} - \frac{\partial B_\zeta}{\partial \rho}\right)$$

$$J^\zeta = \frac{1}{\mu_0\sqrt{g}}\left(\frac{\partial B_\theta}{\partial \rho} - \frac{\partial B_\rho}{\partial \theta}\right)$$

$\mathbf{B}(\rho,\theta,\zeta), \mathbf{J}(\rho,\theta,\zeta)$

$$F_\rho = \sqrt{g}(J^\zeta B^\theta - J^\theta B^\zeta) + p'$$
$$F_\beta = \sqrt{g} J^\rho$$

$\mathbf{F}(\rho,\theta,\zeta)$

R, Z, λ and their derivatives are evaluated on a collocation grid in (ρ,θ,ζ) , then multiplied to calculate **F** on this grid

This leads to a system of equations comprised of the force balance error evaluated at the collocation nodes, which we want to make equal to zero -> Can use root-finding or least-squares to solve

$$\boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$$

x is the spectral coefficients of *R,Z,λ*, which is what we are changing to minimize **f**

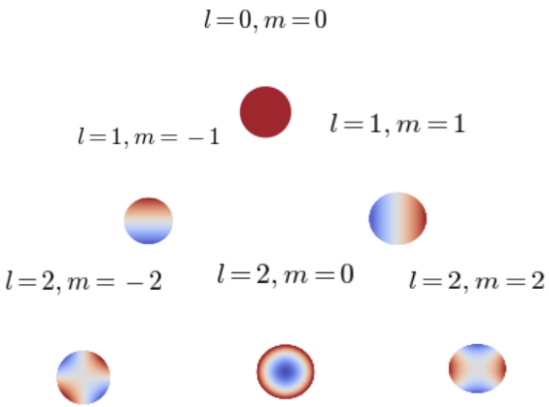
DESC - Fourier-Zernike Spectral Basis

$$R(\rho,\theta,\zeta) = \sum_{m=-M,n=-N,l=0}^{M,N,L} R_{lmn}\mathcal{Z}_l^m(\rho,\theta)\mathcal{F}^n(\zeta)$$

$$\lambda(\rho,\theta,\zeta) = \sum_{m=-M,n=-N,l=0}^{M,N,L} \lambda_{lmn}\mathcal{Z}_l^m(\rho,\theta)\mathcal{F}^n(\zeta)$$

$$Z(\rho,\theta,\zeta) = \sum_{m=-M,n=-N,l=0}^{M,N,L} Z_{lmn}\mathcal{Z}_l^m(\rho,\theta)\mathcal{F}^n(\zeta)$$

Zernike Basis in (*r*,*θ*)



$$\mathcal{Z}_m^l(\rho,\theta) = \begin{cases} \mathcal{R}_l^{|m|}(\rho)cos(|m|\theta) & \text{for } m \geq 0 \\ \mathcal{R}_l^{|m|}(\rho)sin(|m|\theta) & \text{for } m < 0 \end{cases}$$

Zernike Polynomials

Radial Polynomial is of degree *l-2s*, and *l=m,m+2,…, L*

$$\boxed{\mathcal{R}_l^{|m|}(\rho) = \sum_{s=0}^{(l-|m|)/2} \frac{(-1)^s(l-s)!}{s!\,[(l+|m|)/2-s]!\,[(l-|m|)/2+s]!}\rho^{l-2s}}$$

$$\mathcal{F}^n(\zeta) = \begin{cases} cos(|n|N_{FP}\zeta)\text{for } n \geq 0 \\ sin(|n|N_{FP}\zeta)\text{for } n < 0 \end{cases}$$

Toroidal Fourier Series

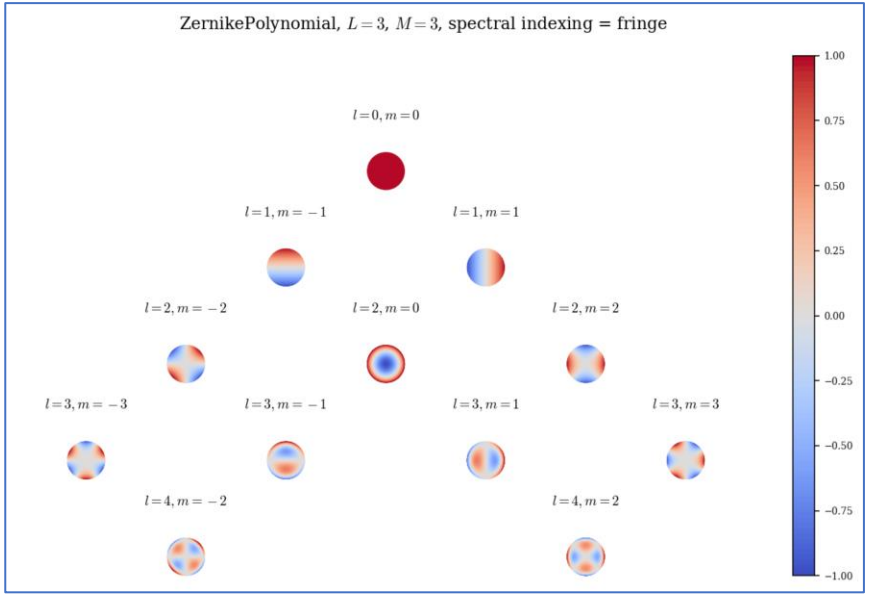
PRINCETON UNIVERSITY

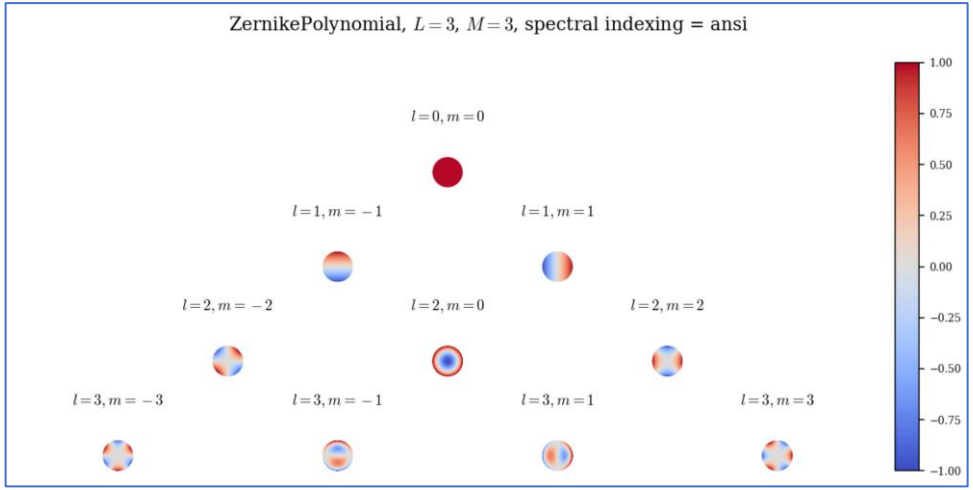
Fringe v Ansi Indexing Scheme

For same L,M, Fringe indexing generally has:

- **More radial resolution (i.e. higher radial degree polynomials)**
- **More modes**

than the corresponding ANSI





DESC Algorithm

Initialization

Inputs
$R_b(\rho = 1, \theta, \zeta)$,
$Z_b(\rho = 1, \theta, \zeta)$,
$p(\rho), \iota(\rho), \psi_a$

Fourier Series
$R_{b,mn}, Z_{b,mn}$

Scale Boundary as Initial Guess for Surface Geometry
$R_{mn}(\rho) \sim \rho R_{b,mn}$
$Z_{mn}(\rho) \sim \rho Z_{b,mn}$

Main Algorithm

Repeat until Desired Resolution

Compute **B** and **J** from
$R(\rho, \theta, \zeta), Z(\rho, \theta, \zeta), \lambda(\rho, \theta, \zeta)$

Compute F_ρ, F_β on collocation grid

$\boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$, use Newton Method to find $\Delta \boldsymbol{x}$

Repeat until converged

Increase Collocation Grid and/or Spectral Resolution

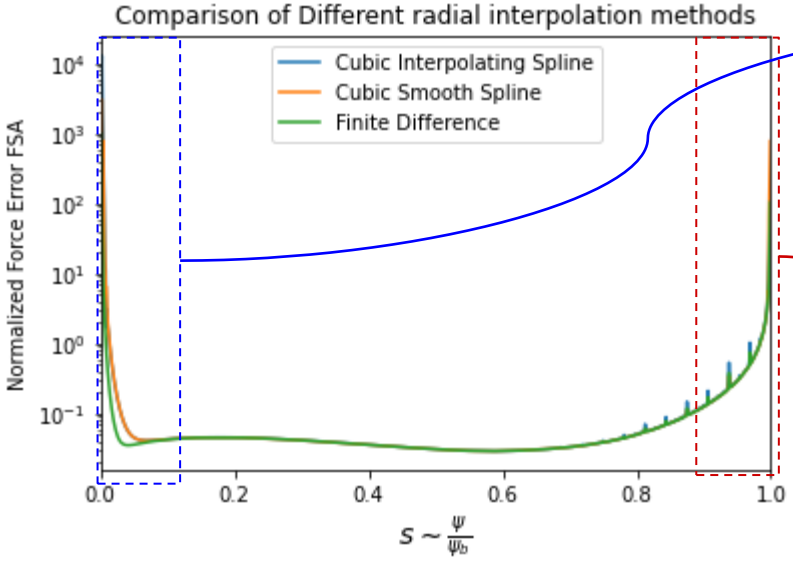
$$R(\rho, \theta, \zeta) = \sum_{m=-M, n=-N, l=0}^{M,N,L} R_{lmn} \mathcal{Z}_l^m(\rho, \theta) \mathcal{F}^n(\zeta)$$

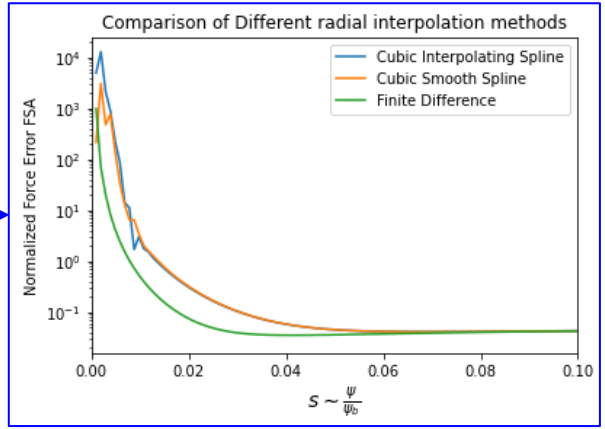
$$\lambda(\rho, \theta, \zeta) = \sum_{m=-M, n=-N, l=0}^{M,N,L} \lambda_{lmn} \mathcal{Z}_l^m(\rho, \theta) \mathcal{F}^n(\zeta)$$

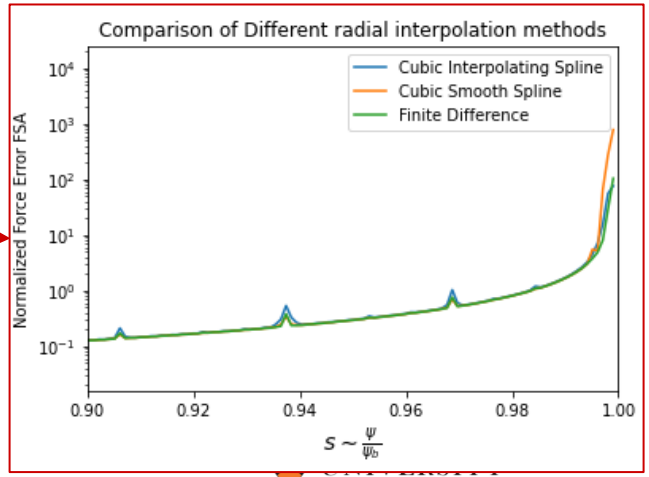
$$Z(\rho, \theta, \zeta) = \sum_{m=-M, n=-N, l=0}^{M,N,L} Z_{lmn} \mathcal{Z}_l^m(\rho, \theta) \mathcal{F}^n(\zeta)$$

$\boldsymbol{x} = [R_{lmn}, Z_{lmn}, \lambda_{lmn}]$

Radial Derivative Method Does Not Affect VMEC Force Error Significantly

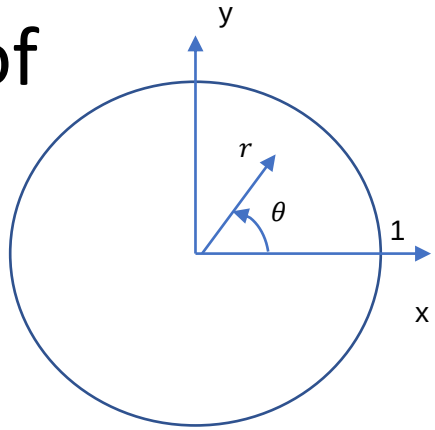






[1](Lewis and Bellan, 1990)

Analyticity Constraint at Polar Axis Proof



- Assume $f(r,\theta)$ is a physical scalar, regular at r=0
- Expand in a Fourier Series: $\sum_{m=-\infty}^{\infty} a_{m(r)} e^{im\theta} \quad = \sum_{-\infty}^{\infty} f_m(r,\theta)$
  - Where the Fourier coefficients are a function of polar radius *r*
- Assume each $f_m(r,\theta)$ is a regular function of *(x,y)* at r=0
- Notice that $e^{im\theta}$ is NOT regular at r=0 (it is multi-valued)
- But, $\left[re^{\pm im\theta}\right]^{|m|} = [x \pm iy]^{|m|}$ is a regular function of (*x*,*y*) b/c it is a <u>polynomial</u> in (*x*,*y*)
- We can rewrite $f(r,\theta)$ as

$$
\begin{aligned}
f_m(r,\theta) &= a_m(r) e^{im\theta} \\
&= \frac{a_m(r)}{r^{|m|}} r^{|m|} e^{i\theta m} \\
&= \frac{a_m(r)}{r^{|m|}} \left[re^{\pm i\theta}\right]^{|m|} \begin{cases} + & m > 0 \\ - & m < 0 \end{cases}
\end{aligned}
$$

Regular at r=0

$$\boxed{f_m(r,\theta)} = \boxed{\frac{a_m(r)}{r^{|m|}}}\boxed{[x \pm iy]^{|m|}}$$

Must be regular at r=0!

Regular at r=0

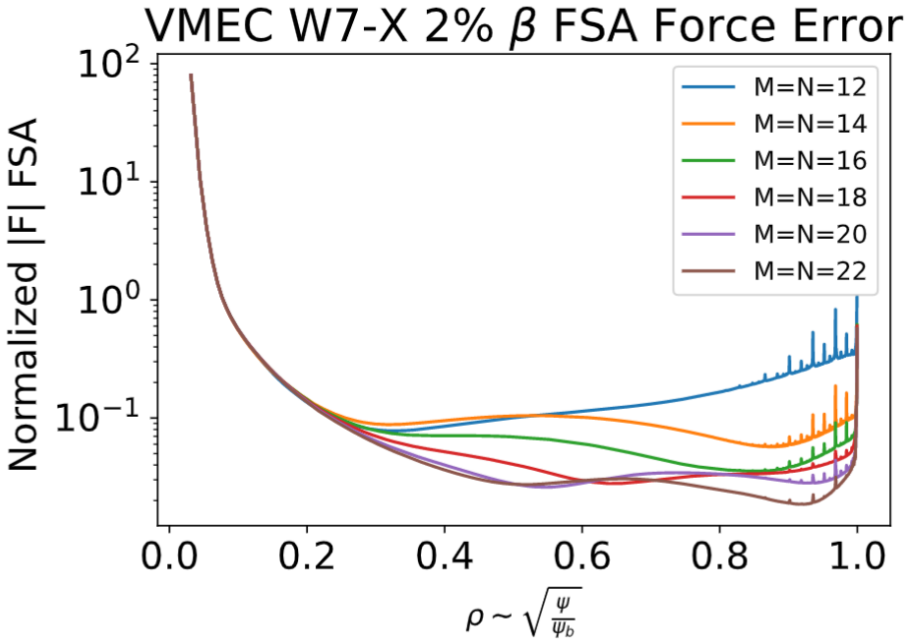
$a_m(r)$ must scale **at least** as $r^{|m|}$

$$\boxed{\lim_{r\to 0} \frac{a_m(r)}{r^{|m|}} < \infty}$$

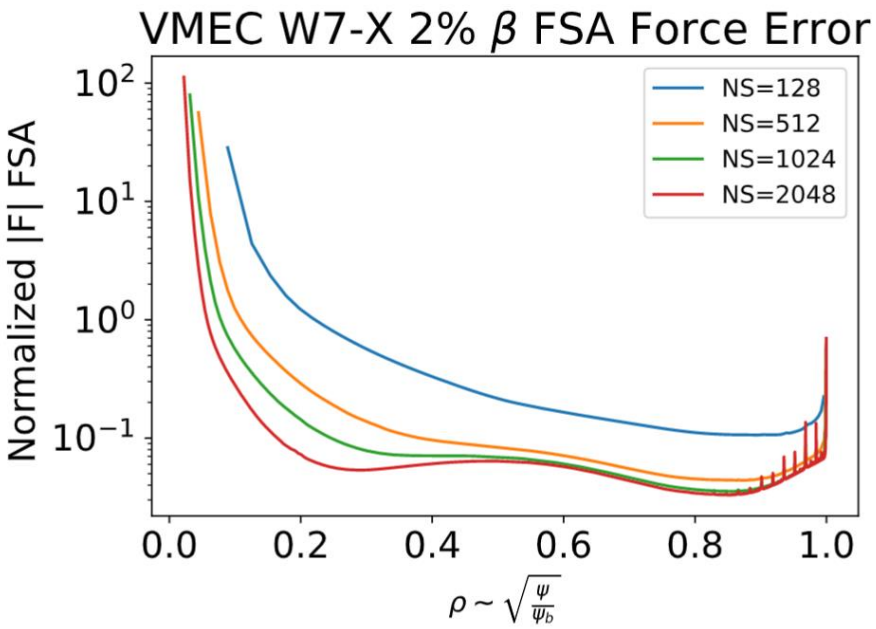
$a_m(r) \sim r^{|m|} + r^{|m|+2} \ldots$

F FSA for Increasing Resolution with VMEC

NS=1024

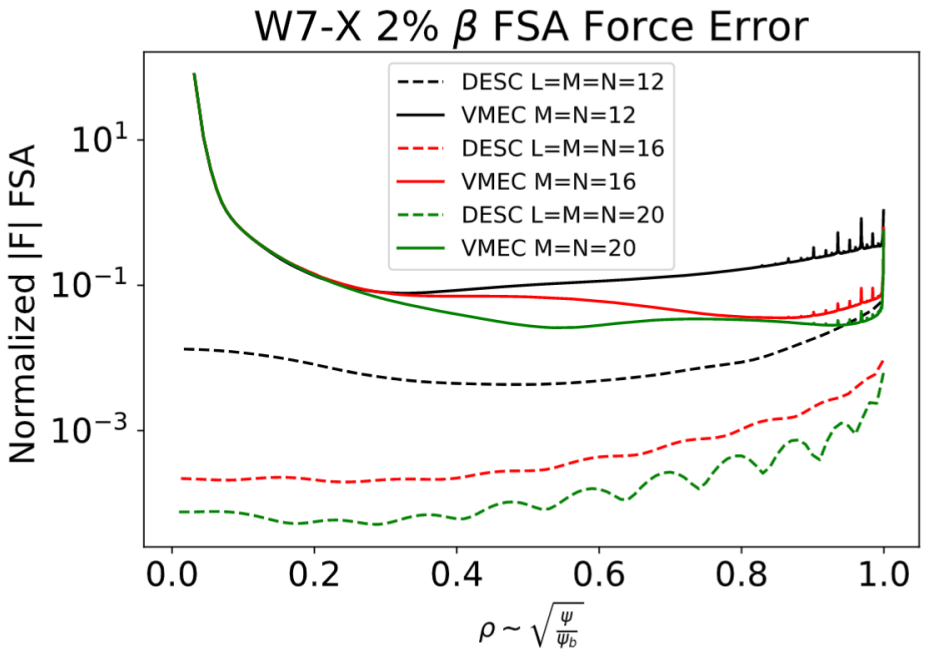


M=N=16



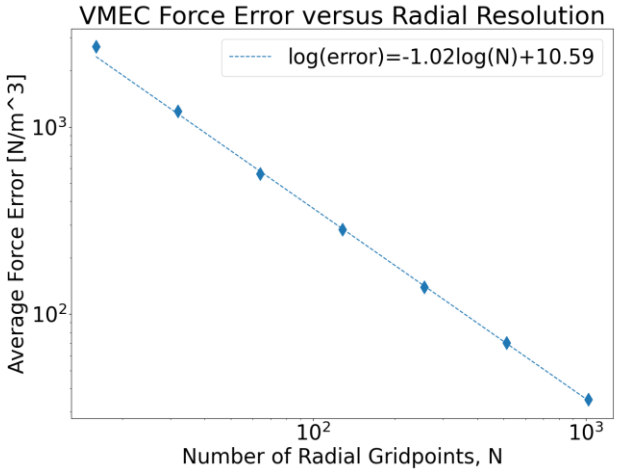
FSA Force Error for Increasing Resolution

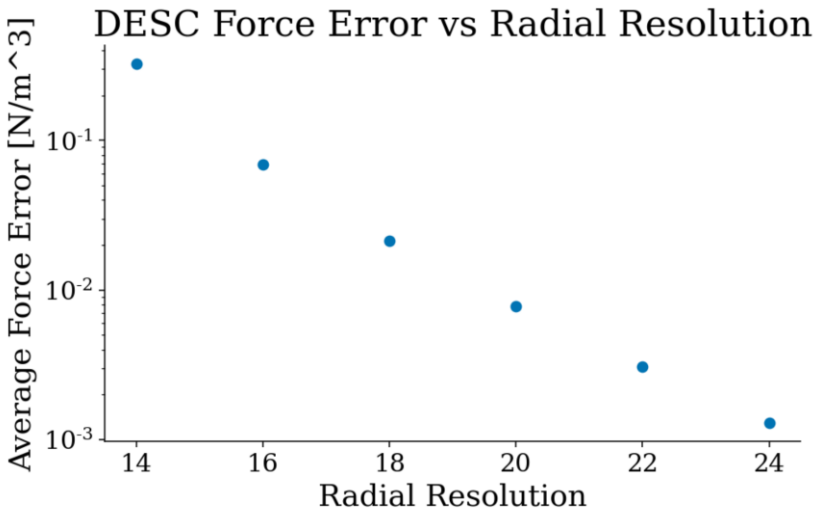
- NS=1024 for the VMEC solutions



DESC compares well to VMEC – Convergence

	Angular Convergence	Radial Convergence
DESC	Exponential	Exponential
VMEC	Exponential	**Algebraic** $\boldsymbol{O}\left(N_{radial}^{-1}\right)$





W7-X Like Equiilbrium