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?

**Plasma Equilibrium**: 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

Stellarator Optimization - VMEC

- 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

\[
\frac{\partial X_{j}^{mn}}{\partial t} = F_{j}^{mn}
\]

\[
W = \int_{V} \left( \frac{B^2}{2\mu_0} + \frac{p}{\gamma - 1} dV \right)
\]

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

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

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

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

\[ F = J \times B - \nabla \rho = 0 \]

(Dudt and Kolemen 2020)

3D Spectral Representation of \( \mathbf{x} = (R, \lambda, Z) \) using Fourier-Zernike Basis
Force Error as an Error Metric

- 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 \( \lambda \) 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

\[
\begin{align*}
\mathbf{e}_s &= \begin{bmatrix} \frac{\partial R}{\partial s} \\ 0 \\ \frac{\partial Z}{\partial s} \end{bmatrix}, \\
\mathbf{e}_u &= \begin{bmatrix} \frac{\partial R}{\partial u} \\ 0 \\ \frac{\partial Z}{\partial u} \end{bmatrix}, \\
\mathbf{e}_v &= \begin{bmatrix} \frac{\partial R}{\partial v} \\ \frac{R}{\partial v} \\ \frac{\partial Z}{\partial v} \end{bmatrix}, \\
\sqrt{g} &= \mathbf{e}_s \cdot \mathbf{e}_u \times \mathbf{e}_v \\
J^s &= \frac{1}{\mu_0 \sqrt{g}} \left( \frac{\partial B_u}{\partial u} - \frac{\partial B_v}{\partial v} \right), \\
J^u &= \frac{1}{\mu_0 \sqrt{g}} \left( \frac{\partial B_s}{\partial v} - \frac{\partial B_v}{\partial s} \right), \\
J^v &= \frac{1}{\mu_0 \sqrt{g}} \left( \frac{\partial B_u}{\partial s} - \frac{\partial B_s}{\partial u} \right), \\
\mathbf{B}(s, u, v), \mathbf{J}(s, u, v) \\
F_a &= \sqrt{g} (J^v B^u - J^u B^v) + p' \\
F_\beta &= J^s
\end{align*}
\]
Force Error Metrics

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

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

- **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**

  $$< |\nabla p| >_{vol} = \frac{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \int_{s=0}^{1} |\nabla p| \sqrt{g} |dsd\phi d\theta}{\int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \int_{s=0}^{1} \sqrt{g} |dsd\phi d\theta}$$
Calculated Force Error Insensitive to Radial Derivative Method

Only near-axis changes significantly with method

2\textsuperscript{nd} Order Central Differences used for remainder of results shown in this presentation

VMEC W7-X 2\% $\beta$ FSA Force Error

Normalized $|F|/FSA$

$\rho \sim \sqrt{\frac{\psi}{\psi_0}}$

2\textsuperscript{nd} Order Central Difference
4\textsuperscript{th} Order Central Difference
Cubic Interpolating Spline
Quintic Interpolating Spline
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.

<table>
<thead>
<tr>
<th>Angular Resolution</th>
<th>Radial Resolution</th>
<th>Other Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>DESC</td>
<td>M=N=[8,10,12,14,16,18,20]</td>
<td>L=M=N</td>
</tr>
<tr>
<td>VMEC</td>
<td>M=N=[8,10,12,14,16,18,20]</td>
<td>NS=[256,512,1024]</td>
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Solution Comparison - Flux Surfaces Indistinguishable by Eye
For Given Resolution, DESC has lower Force Error

<table>
<thead>
<tr>
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<th>W7X M=N=12</th>
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<tr>
<td>Energy (J)</td>
<td>$8.4648759e+07$</td>
</tr>
<tr>
<td>$</td>
<td>F</td>
</tr>
<tr>
<td>Runtime (1 CPU)</td>
<td>0.71 hours</td>
</tr>
<tr>
<td>DESC (L=12)</td>
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W7X Beta = 2% Force Error versus Resolution

![Graph showing W7X Beta = 2% Force Error versus Resolution](image-url)
For Given Time to Solution, DESC has lower Force Error

| W7X M=N=12 | Energy (J) | $|\mathbf{F}|/|\nabla \rho|$ | 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 |

$\langle F \rangle_{vol} = \frac{\int_{0}^{2\pi} \int_{0}^{2\pi} \int_{0}^{0.99} \frac{|\mathbf{F}|}{\sqrt{g}} d\rho d\phi d\theta}{\int_{0}^{2\pi} \int_{0}^{2\pi} \int_{0}^{0.99} \sqrt{g} d\rho d\phi d\theta}$
VMEC Force Error is Noticeably Higher Near-axis

- This could be due to VMEC’s Fourier coefficients not explicitly obeying analyticity constraint near axis.
Analyticity Constraints for Functions in Polar Domains

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

\[
\lim_{\rho \to 0} \frac{a_m}{\rho^m} < \infty \quad \lim_{\rho \to 0} \frac{b_m}{\rho^m} < \infty
\]

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

\(^{(1)}\text{(Lewis and Bellan, 1990)}\)
Analytic Constraint Near Axis

- Fourier coefficients of an analytic function must scale as $\rho^m$ 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!

Flux-Surface Averaged Force Error vs Radius
Both DESC and VMEC Poloidal Angle are Optimal

- Spectral condensation as defined by Hirshman and Meier (1985)
  \[ M(p,q) = \frac{\sum_{m=1}^q m^2 S_p(m)}{\sum_{m=1}^q S_p(m)} \]

- 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)

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VMEC Force Error versus Radial Resolution

DESC Force Error vs Radial Resolution
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!
Repository: https://github.com/PlasmaControl/DESC
Python Package: pip install desc-opt
What DESC Solves

**Inputs:** $R_b(\theta, \zeta), Z_b(\theta, \zeta), p(\rho), \iota(\rho)$

\[ R = \begin{bmatrix} \frac{\partial R}{\partial \rho} \\ 0 \end{bmatrix}, \quad \mathbf{e}_\rho = \sqrt{g} = \mathbf{e}_\rho \cdot \mathbf{e}_\Theta \times \mathbf{e}_\zeta \]

\[ B^\Theta = \frac{\psi'}{\sqrt{g}} \left( 1 + \frac{\partial \lambda}{\partial \Theta} \right) \]

\[ B^\zeta = \frac{1}{\sqrt{g}} \psi' \left( 1 + \frac{\partial \lambda}{\partial \zeta} \right) \]

\[ J^\rho = \frac{1}{\mu_0 \sqrt{g}} \left( \frac{\partial B^\zeta}{\partial \Theta} - \frac{\partial B^\Theta}{\partial \zeta} \right) \]

\[ J^\Theta = \frac{1}{\mu_0 \sqrt{g}} \left( \frac{\partial B^\rho}{\partial \Theta} - \frac{\partial B^\Theta}{\partial \rho} \right) \]

\[ J^\zeta = \frac{1}{\mu_0 \sqrt{g}} \left( \frac{\partial B^\Theta}{\partial \zeta} - \frac{\partial B^\zeta}{\partial \rho} \right) \]

**B(\rho, \theta, \zeta), J(\rho, \theta, \zeta)**

\[ F_\rho = \sqrt{g}(J^\zeta B^\Theta - J^\Theta B^\zeta) + p' \]

\[ F_\beta = \sqrt{g} J^\rho \]

**F(\rho, \theta, \zeta)**

\[ f(x) = 0 \]

\[ x \text{ is the spectral coefficients of } R, Z, \lambda, \text{ which is what we are changing to minimize } f \]

$R, Z, \lambda$ and their derivatives are evaluated on a collocation grid in $(\rho, \theta, \zeta)$, 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.
DESC - Fourier-Zernike Spectral Basis

\[ R(\rho, \theta, \zeta) = \sum_{m=-M,n=-N,l=0}^{M,N,L} R_{lmn} Z_l^m(\rho, \theta) F^n(\zeta) \]

\[ \lambda(\rho, \theta, \zeta) = \sum_{m=-M,n=-N,l=0}^{M,N,L} \lambda_{lmn} Z_l^m(\rho, \theta) F^n(\zeta) \]

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

\[ Z_l^m(\rho, \theta) = \begin{cases} \mathcal{R}_l^{|m|}(\rho) \cos(|m|\theta) & \text{for } m \geq 0 \\ \mathcal{R}_l^{|m|}(\rho) \sin(|m|\theta) & \text{for } m < 0 \end{cases} \]

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

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

Zernike Basis in \((r,\theta)\)

- \(l=0, m=0\)
- \(l=1, m=-1\)
- \(l=1, m=1\)
- \(l=2, m=-2\)
- \(l=2, m=0\)
- \(l=2, m=2\)

Zernike Polynomials

Radial Polynomial is of degree \(l-2s\), and \(l=m,m+2,\ldots, L\)

Toroidal Fourier Series
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
\[ R_b(\rho = 1, \theta, \zeta), \]
\[ Z_b(\rho = 1, \theta, \zeta), \]
\[ p(\rho), \psi_a(\rho), \phi(\rho), \psi_a \]

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

Fourier Series
\[ R_{b,mn}, Z_{b,mn} \]

Main Algorithm

Repeat until Desired Resolution

Compute \( B \) and \( J \) from
\[ R(\rho, \theta, \zeta), Z(\rho, \theta, \zeta), \lambda(\rho, \theta, \zeta) \]

Repeat until Desired Resolution

Increase Collocation Grid and/or Spectral Resolution

\[ f(x) = 0, \text{ use Newton Method to find } \Delta x \]

Repeat until converged

\[ x = [R_{lmn}, Z_{lmn}, \lambda_{lmn}] \]
Radial Derivative Method Does Not Affect VMEC Force Error Significantly
Analyticity Constraint at Polar Axis Proof

- Assume \( f(r, \theta) \) is a physical scalar, regular at \( r=0 \)
- Expand in a Fourier Series: \( \sum_{m=-\infty}^{\infty} a_m(r)e^{im\theta} = \sum_{m=-\infty}^{\infty} f_m(r, \theta) \)
  - 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, \([re^{\pm im\theta}]^{|m|} = [x \pm iy]^{|m|}\) is a regular function of \((x,y)\) b/c it is a polynomial in \((x,y)\)
- We can rewrite \( f(r, \theta) \) as

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

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

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

\[
a_m(r) \sim r^{|m|} + r^{|m|+2} \ldots
\]
F FSA for Increasing Resolution with VMEC

VMEC W7-X 2% $\beta$ FSA Force Error

Normalized $|F|$ FSA

$\rho \sim \sqrt{\frac{\psi}{\psi_0}}$

NS=1024

M=N=16

VMEC W7-X 2% $\beta$ FSA Force Error

Normalized $|F|$ FSA

$\rho \sim \sqrt{\frac{\psi}{\psi_0}}$

NS=128
NS=512
NS=1024
NS=2048
FSA Force Error for Increasing Resolution

- NS=1024 for the VMEC solutions
DESC compares well to VMEC – Convergence

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### Diagrams

1. **VMEC Force Error versus Radial Resolution**
   - The graph shows the log-log plot of average force error versus radial resolution.
   - The equation $\log(\text{error}) = -1.02\log(N) + 10.59$ fits the data.

2. **DESC Force Error vs Radial Resolution**
   - The graph illustrates the force error for different radial resolutions.
   - The error decreases as the radial resolution increases.
W7-X Like Equilibrium