Application of SIESTA to Island Formation in HSX

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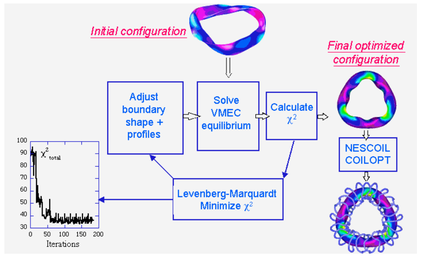
Overview

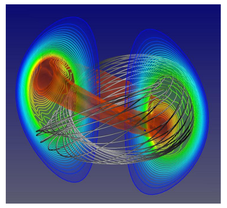
- SIESTA (Scalable Iterative Equilibrium Solver for Toroidal Applications) is a 3D ideal MHD equilibrium solver capable of resolving islands and stochastic regions in an accurate and scalable manner
- The VMEC output is used as the initial equilibrium which is perturbed using the nonlinear energy minimization procedures of SIESTA
- Simulations on HSX configurations are being done in order to analyze code resolution of islands in stellarators
- Large, complicated mode structure from helical shaping in HSX requires at least 10 poloidal and 10 toroidal Fourier modes to be included in SIESTA runs
- A pentadiagonal solver is being tested and implemented to improve convergence of the code on HSX and other devices with complex geometry/Fourier spectrums
- This work will be a precursor to implementation in stellarator optimization suites, for study of new concepts

Introduction to SIESTA

A fast (~mins), scalable 3D MHD-equilibrium solver that resolves magnetic islands and stochastic regions would be useful for numerous applications

- STELLARATOR OPTIMIZATION.- include in optimization procedure at run-time (i.e., in STELLOPT suite).
- STELLARATOR/3D TOKAMAK EQUILIBRIUM RECONSTRUCTION.- (J. D. Hanson, V3FIT).
- EXTENDED-MHD SIMULATIONS.- initialize MHD simulations of neoclassical tearing modes at ITER-relevant resolutions.

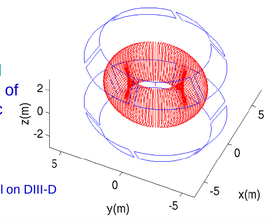




[Source: CEMM, PPPL]

Extended MHD simulation

- EXPERIMENT DESIGN and INTERPRETATION.- control of ELMs via resonant magnetic perturbations?



ELMs control on DIII-D

GUIDING PRINCIPLES.- avoid integration along magnetic field lines (slow/inaccurate) and retain scalability (to parallel environments). Also, build on previous ORNL expertise with 3D MHD codes (VMEC, COBRA…)

Basic Equations of SIESTA

Ideal MHD energy (target function for minimization):

$$W = \int \frac{B^2}{2\mu_o} + \frac{p}{\gamma - 1} dVol$$

The force in the unperturbed state is given by:

$$\vec{F} = \mu_o^{-1}(\nabla \times \vec{B}) \times \vec{B} - \nabla p$$

For any plasma displacement, conservation of magnetic flux and mass requires:

$$\delta\vec{B}(\vec{\xi}) = \nabla \times (\vec{\xi} \times \vec{B}) \quad \text{Faraday's law}$$

$$\delta p(\vec{\xi}) = -\vec{\xi} \cdot \nabla p - \gamma p \nabla \cdot \vec{\xi} \quad \text{Mass conservation}$$

The force in the "displaced" state is given by:

$$\vec{F} + \delta\vec{F}(\vec{\xi}) = \mu_o^{-1}(\nabla \times (\vec{B} + \delta\vec{B}(\vec{\xi})) \times (\vec{B} + \delta\vec{B}(\vec{\xi})) - \nabla(p + \delta p(\vec{\xi}))$$

To find equilibrium, solve nonlinear equation $\vec{F}_{tot} = \vec{F} + \delta\vec{F}(\vec{\xi}) = \vec{0}$ and update fields.

SIESTA uses a hybrid spectral/finite differencing representation of the fields in terms of the VMEC coordinates as follows:

$$B^\alpha(\rho,\theta,\phi) = \sum_{m=0}^{mpol} \sum_{n=-ntor}^{ntor} (B^\alpha)^c_{mn}(\rho)\cos(m\theta + n\phi) + (B^\alpha)^s_{mn}(\rho)\sin(m\theta + n\phi)$$

$$p(\rho,\theta,\phi) = \sum_{m=0}^{mpol} \sum_{n=-ntor}^{ntor} p^c_{mn}(\rho)\cos(m\theta + n\phi) + p^s_{mn}(\rho)\sin(m\theta + n\phi)$$

Since highest order radial derivative is second order, the resulting Hessian matrix is block tridiagonal. This lends itself to fast, optimized solvers, such as BCYCLIC.

Finding the SIESTA Equilibrium

SIESTA solves for the ideal MHD equilibrium using Newton's Method, a nonlinear optimization algorithm. Using this method, the energy is approximated locally as a quadratic function, obtained from the Taylor series expansion of the energy function.

$$\hat{W} = W_k + \nabla W_k \delta\vec{\xi}_{k+1} + \frac{1}{2}\delta\vec{\xi}^T_{k+1} \nabla^2 W_k \delta\vec{\xi}_{k+1}$$

$$\min \hat{W} \Leftrightarrow \nabla^2 W_k \delta\vec{\xi}_{k+1} = -\nabla W_k$$

The local quadratic approximation to the energy function has been made. Since the first derivative of the energy is the force and the second derivative is the Hessian of our function, this can be rewritten as:

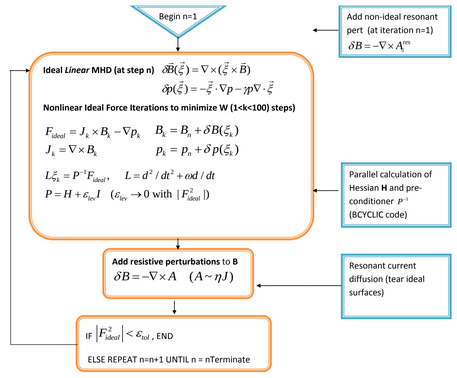
$$H_k \delta\vec{\xi}_{k+1} = -F_k$$

Then find new displacement as follows:

$$\vec{\xi}_{k+1} = \vec{\xi}_k + \delta\vec{\xi}_{k+1}$$

Beginning with a converged VMEC solution gives an equilibrium starting configuration. This stationary point is potentially unstable. Applying an initial resonant perturbation at the lowest-order rational surfaces may lead to island formation and a lower energy equilibrium. This is how the simulation is started.

At each iteration of the nonlinear Newton's method, the above linear equation must be solved. This amounts to inverting a tridiagonal Hessian matrix. Iterative solvers such as GMRES and variants of conjugate gradient work best for this, due to the large condition number of the Hessian.



Levenberg-Marquardt Technique and Pentadiagonal Solver

The Levenberg-Marquardt technique is used to ensure that the Hessian matrix is positive-definite, which is required for a decrease of the linearized energy at each iteration. Solving the linear problems more efficiently leads to faster convergence of the overall nonlinear problem. The eigenvalues of the Hessian matrix are both positive and negative, corresponding to stable and unstable modes. The current working version of SIESTA uses a block tridiagonal solver which approximates the Levenberg-Marquardt technique as follows:

$$H_k \delta\vec{\xi}_{k+1} = -\vec{F}_k \to (H_k + \mu_k I)\delta\vec{\xi}_{k+1} = -\vec{F}_k$$

This shifts the eigenvalue spectrum completely to the positive side if done correctly. This results in a positive definite Hessian matrix.

The difficulty is in choosing the LM parameter such that the spectrum shifts completely to one side of 0. The full Levenberg-Marquardt technique is being implemented so that there is no guessing which parameter to pick. This is accomplished by first squaring the Hessian and then adding the LM parameter, thus ensuring positive-definiteness:

$$(H^T_k H_k + \mu_k I)\delta\vec{\xi}_{k+1} = -H^T_k \vec{F}_k$$

$$\kappa = \frac{\lambda_{\max}}{\lambda_{\min}} \to \kappa = \frac{\lambda^2_{\max} + \mu_k}{\lambda^2_{\min} + \mu_k}$$

Note that a smart choice of the LM parameter can now be used not only to guarantee the system is positive definite, but also to reduce the condition number. This will decrease the number of iterations required to solve the linear problem.

Squaring the Hessian changes the structure to block pentadiagonal. This requires a different solver, which has already been written implementing the Thomas algorithm. This full LM technique should greatly improve convergence, and is currently being implemented into the code.

Thomas Algorithm

The Thomas Algorithm is a method to efficiently factor and invert a block diagonal matrix; in this case a block pentadiagonal matrix.

$$\begin{pmatrix} a_1 & b_1^+ & c_1^+ & 0 & 0 & 0 & 0 \\ b_2^- & a_2 & b_2^+ & c_2^+ & . & . & 0 \\ c_3^- & b_3^- & a_3 & b_3^+ & c_3^+ & . & 0 \\ 0 & c_4^- & b_4^- & a_4 & b_4^+ & c_4^+ & 0 \\ 0 & . & . & . & . & . & . \\ 0 & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & c_N^- & b_N^- & a_N \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{pmatrix} = \begin{pmatrix} s_1 \\ s_2 \\ . \\ . \\ . \\ s_N \end{pmatrix}$$

This can be solved starting with the following equation

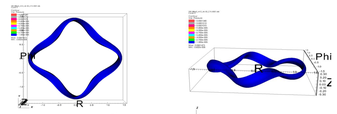
$$x_N = a_N^{-1}(s_N - b_N^- \cdot x_{N-1} - c_N^- \cdot x_{N-2})$$

Island Formation in HSX

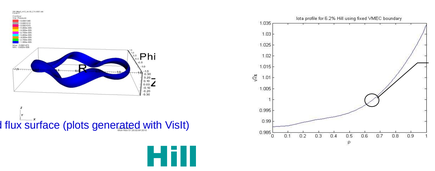
HSX is a 4 field-period, quasi-helically symmetric stellarator located at the University of Wisconsin-Madison. Due to the distinctive, strong helical shaping, more modes (particularly toroidal modes) are required to resolve islands using SIESTA. A perturbed tokamak, for example, can be simulated using fewer modes.

- Configurations studied chosen for resonant iota and size of islands
- Islands were previously observed in Biot-Savart field-line following
- Hill configuration shows large 4/4 (m=4, n=4) island chain
- Well configuration shows somewhat smaller 8/7 (m=7, n=8) island chain

4/4 surface is lowest rational found in HSX



Strong helical shaping of HSX outermost closed flux surface (plots generated with VisIt)



Add 4/4 perturbation here

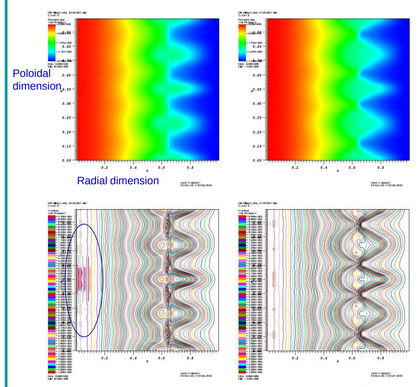
Hill

4/4 (m=4, n=4) Island formation evolves by including more modes

- Axis has a lot of spectral content
- Islands get wider, pressures relax as more modes are included

Below plots are in SIESTA curvilinear coordinates at constant toroidal angle

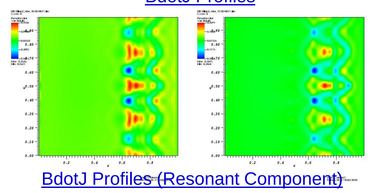
Pressure Profiles



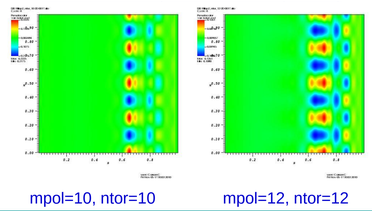
mpol=10, ntor=10 mpol=12, ntor=12

Pressure doublets are slowly resolved by including more m/n modes that are resonant with the safety factor (iota) of the rational surface!

BdotJ Profiles



BdotJ Profiles (Resonant Component)

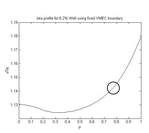


mpol=10, ntor=10 mpol=12, ntor=12

4/4, 8/8 resonances included in left simulation; 4/4, 8/8, 12/12 resonances included in right simulation

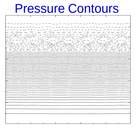
Well

8/7 surface is lowest rational found in 6.2% Well



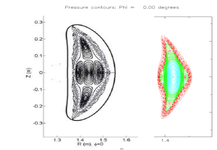
radial

Pressure Contours



poloidal

Smaller island size and larger mode content of Well case makes it difficult to converge on an island solution.



Vacuum field-line following vs. SIESTA pressure contours. A qualitative look. (field-line following from Gerhardt thesis)

Summary

- 4/4 island chain requires at least m=10, n=10 modes for resolution of islands.
- 8/7 island chain in Well requires more modes (m=10, n~20) currently to start to see island formation.
- Several multiples of resonant m/n are required for flattening of pressure profiles within islands.
- Implementation of pentadiagonal solver should improve convergence of SIESTA, yielding better results for stellarator applications.

References

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3. S. Gerhardt thesis, University of Wisconsin-Madison (2004)
4. S.P. Hirshman, H.K. Meier, *Phys. Fluids* 28 (5), (1985)

Thanks to J. Schmitt for lots of VMEC help!

This research was supported in part by an award from the Department of Energy (DOE) Office of Science Graduate Fellowship Program (DOE SCGF). The DOE SCGF Program was made possible in part by the American Recovery and Reinvestment Act of 2009. The DOE SCGF program is administered by the Oak Ridge Institute for Science and Education for the DOE. ORISE is managed by Oak Ridge Associated Universities (ORAU) under DOE contract number DE-AC05-06OR23100. All opinions expressed in this paper are the author's and do not necessarily reflect the policies and views of DOE, ORAU, or ORISE.

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