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### Benchmarking

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#### **MDC-2 Benchmarking of kinetic models: overview & steps**

- Codes: HAGIS, MARS-K, MISK
- Choice of equilibria for benchmarking
  - Start by using Solov'ev

**Spring 2011** 

- HAGIS / MARS-K, and MISK / MARS-K benchmarked to different degrees using Solov'ev equilibria; collect/cross compare results
  - HAGIS/MARS results published [Y. Liu et al., Phys. Plasmas 15, 112503 (2008)]
- Simplicity may lead to unrealistic anomalies better to use realistic cases?
- Move on to ITER-relevant equilibria
  - Use Scenario IV, or new equilibria recently generated for WG7 task by Y. Liu (more realistic; directly applicable to ITER)
  - Need kinetic profiles as well as fluid pressure
- Approach to stability comparison start with
  - ideal fluid quantities ( $\delta W^{no-wall}$ ,  $\delta W^{wall}$ , etc.)
  - n = 1 (consider n > 1 in a future step)
  - perturbative approach on static eigenfunction input ensure that unstable eigenfunction is consistent among codes (e.g. no-wall ideal for MISHKA)
  - no-wall / with-wall  $β_N$  limits (equilibrium β scan needed)

Fall 2011

## Initial comparison of stability calculations for Solov'ev, ITER cases (Oct. 2011)

Work in progress!

	r <sub>wall</sub> /a	ldeal δW /(-δW <sub>∞</sub> )	Re(δW <sub>K</sub> ) /(-δW <sub>∞</sub> )	Im(δW <sub>κ</sub> ) /(-δW <sub>∞</sub> )	γτ <sub>w</sub>	ωτ <sub>w</sub>	$\delta W_{K}$ /(- $\delta W_{\infty}$ ) ( $\omega_{E} \rightarrow \infty$ )
<u>Solov'ev 1</u> (MARS-K) (MISK)	1.15	1.187 1.122	0.0256 0.0243	-0.0121 0.0280	0.804 0.850	-0.0180 -0.0452	0.157 0.236
<u>Solov'ev 3</u> (MARS-K) (MISK)	1.10	1.830 2.337	0.208 0.371	-0.343 0.060	0.350 0.232	-0.228 -0.027	0.689
<u>ITER</u> (MARS-K) (MISK)	1.50	0.682 0.677	141.5 0.665	2.286 -0.548	-0.988 0.071	0.00019 0.437	8.46

- Calculations from MISK, and MARS-K (perturbative)
  - Good agreement on ideal  $\delta W$ , Solov'ev 1 Re( $\delta W_{K}$ ),  $\gamma \tau_{w}$
  - Less agreement on Solov'ev 3, ωτ<sub>w</sub>
  - Very different ITER result (do we have different input?)

## We have compared results for Solov'ev 1 case broken down into particle types, and they do not agree.

MISK now has the ability to separate I=0 and  $I\neq 0$  components.

	thermal ions						thermal electrons		Alfvén Laver		Total	
	trapped				circulating		trapped $(l = 0 \text{ only})$		Aliven Layer		Iotai	
	$l = 0$ $l \neq 0$		4 0	circulating		$\operatorname{crapped}(t = 0 \operatorname{orm} y)$						
	real	imag	real	imag	real	imag	real	imag	real	imag	real	imag
Solov'ev 1	$8.46 \times 10^{-2}$	$-1.48 \times 10^{-2}$	$3.10 \times 10^{-3}$	$\!$	$-2.10 \times 10^{-3}$	$-1.33 \times 10^{-4}$	$-6.00 \times 10^{-2}$	$2.95\!\times\!10^{3}$			$2.56\!\times\!10^{\text{-}2}$	$-1.21 \times 10^{-2}$
50107 67 1	$1.45{\times}10^{\text{-2}}$	$2.23\!\times\!\!10^{\text{-}6}$	$3.84 \times 10^{-3}$	$8.12 \times 10^{-3}$	$-8.90 \times 10^{-3}$	$2.05\!\times\!10^{\text{-}2}$	$1.58\!\times\!10^{\text{-}2}$	$3.68\!\times\!10^{\text{-}5}$	0	0	$2.51\!\times\!10^{\text{-}2}$	$2.87{\times}10^{-2}$
Soloviev 3											$2.08\!\times\!10^{\text{-}1}$	$-3.43 \times 10^{-1}$
50107 67 5	$1.90{\times}10^{\text{-}1}$	$2.50{\times}10^{-6}$	$-8.69 \times 10^{-3}$	$1.45{\times}10^{\text{-}2}$	$4.03\!\times\!10^{\text{-}3}$	$3.93\!\times\!10^{-2}$	$1.90{\times}10^{\text{-}1}$	$6.46\!\times\!10^{-5}$	$-3.81 \times 10^{-5}$	$\text{-}1.20{\times}10^{\text{-}5}$	$3.71\!\times\!10^{-1}$	$1.46{ imes}10^{-2}$
ITER												
m	$8.52 \times 10^{-1}$	$3.05 \times 10^{-4}$	$-9.96 \times 10^{-2}$	$2.68 \times 10^{-2}$	$-2.23 \times 10^{-1}$	$3.78 \times 10^{-2}$	$1.35 \times 10^{-1}$	$-1.64 \times 10^{-2}$	$-1.03 \times 10^{-2}$	$-7.95 \times 10^{-1}$	$6.53 \times 10^{-1}$	$-7.46 \times 10^{-1}$

 $\delta W_{\rm K}$ /- $\delta W_{\rm w}$  for MISK (blue) and MARS-K (red)

### MISK frequency calculation improved by analytic calculation of integrals involving $1/v_{||}$ at $v_{||} \rightarrow 0$ . Note: does not affect the outcome very much.



**WNSTX-U** 

## MISK calculates the energy integral numerically, MARS-K does it analytically

$$I_{\varepsilon}\left(\Psi,\Lambda,l\right) = \int_{0}^{\infty} \frac{n\left(\omega_{*N} + \left(\hat{\varepsilon} - \frac{3}{2}\right)\omega_{*T}\right) + n\omega_{E} - \omega_{r} - i\gamma}{n\left(\omega_{D} + \left(l + \alpha nq\right)\omega_{b}\right) - i\nu_{\text{eff}} + n\omega_{E} - \omega_{r} - i\gamma}\hat{\varepsilon}^{\frac{5}{2}}e^{-\hat{\varepsilon}}d\hat{\varepsilon}.$$

#### Analytical solutions are only possible in certain cases:

#### 2. $\nu_{\text{eff}} = \text{constant}$ (no energy dependence), and l = 0 for trapped particles

This is the case for trapped particles without energy-dependent collisions, with only the precession drift and no bounce frequency,

$$I_{\varepsilon} = \int_{0}^{\infty} \frac{\Omega_{*}^{a} + \Omega_{n} + \hat{\varepsilon} \Omega_{*}^{b}}{\hat{\varepsilon} + \Omega_{n}} \hat{\varepsilon}^{\frac{5}{2}} e^{-\hat{\varepsilon}} d\hat{\varepsilon}, \qquad (39)$$

where  $\Omega_n = (n\omega_E - \omega - i\nu_{\text{eff}})/(n\overline{\omega_D})$ ,  $\Omega^a_* = (n\omega_{*N} - \frac{3}{2}n\omega_{*T} + i\nu_{\text{eff}})/(n\overline{\omega_D})$ ,  $\Omega^b_* = \omega_{*T}/\overline{\omega_D}$ , and  $\omega_D = \overline{\omega_D}\hat{\varepsilon}$  (ie.  $\overline{\omega_D}$  is the non-energy dependent portion of  $\omega_D$ ). The solution is given in Ref. [16], Eq. 30:

$$I_{\varepsilon} = \frac{15\sqrt{\pi}}{8}\Omega^b_* + 2\sqrt{\pi}\left(\Omega_n + \Omega^a_* - \Omega_n\Omega^b_*\right) \left[\frac{3}{8} - \frac{1}{4}\Omega_n + \frac{1}{2}\Omega^2_n + i\frac{1}{2}\Omega^{\frac{5}{2}}_n Z\left(i\Omega^{\frac{1}{2}}_n\right)\right],\tag{40}$$

where Z is the plasma dispersion function.



### MISK calculates the energy integral numerically, MARS-K does it analytically (cont.)

$$I_{\varepsilon}\left(\Psi,\Lambda,l\right) = \int_{0}^{\infty} \frac{n\left(\omega_{*N} + \left(\hat{\varepsilon} - \frac{3}{2}\right)\omega_{*T}\right) + n\omega_{E} - \omega_{r} - i\gamma}{n\left(\omega_{D} + \left(l + \alpha nq\right)\omega_{b}\right) - i\nu_{\text{eff}} + n\omega_{E} - \omega_{r} - i\gamma}\hat{\varepsilon}^{\frac{5}{2}}e^{-\hat{\varepsilon}}d\hat{\varepsilon}.$$

#### Analytical solutions are only possible in certain cases:

3.  $\nu_{\text{eff}} = \text{constant}$  (no energy dependence),  $l \neq 0$  for trapped particles, and  $|\omega_D| \ll |l\omega_b|$ 

This is the case again without energy-dependent collisions, for trapped particles with  $l \neq 0$  where the precession drift frequency is neglected with respect to the bounce frequency. If we now define  $\Omega_{n2} = (n\omega_E - \omega - i\nu_{\text{eff}})/(nl\overline{\omega_b})$ ,  $\Omega_*^{a2} = (n\omega_{*N} - \frac{3}{2}n\omega_{*T} + i\nu_{\text{eff}})/(nl\overline{\omega_b})$ ,  $\Omega_*^{b2} = \omega_{*T}/\overline{l\omega_b}$ , and  $\omega_b = \overline{\omega_b}\hat{\varepsilon}^{\frac{1}{2}}$  (ie.  $\overline{\omega_b}$  is the non-energy dependent portion of  $\omega_b$ ), then

$$I_{\varepsilon} = \int_{0}^{\infty} \frac{\Omega_{*}^{a2} + \Omega_{n2} + \hat{\varepsilon} \Omega_{*}^{b2}}{\frac{\overline{\omega_{D}}}{l\omega_{b}} \hat{\varepsilon} + \hat{\varepsilon}^{\frac{1}{2}} + \Omega_{n2}} \hat{\varepsilon}^{\frac{5}{2}} e^{-\hat{\varepsilon}} d\hat{\varepsilon}.$$
(43)

With  $\overline{\omega_D}/l\overline{\omega_b} \to 0$  this has the analytical solution

$$I_{\varepsilon} = -\Omega_{*}^{b2} \left( \frac{15\sqrt{\pi}}{8} \Omega_{n2} - 6 \right) + 2\sqrt{\pi} \left( \Omega_{n2} + \Omega_{*}^{a2} + \Omega_{n2}^{2} \Omega_{*}^{b2} \right) \left[ -\Omega_{n2} \left( \frac{3}{8} + \frac{1}{4} \Omega_{n2}^{2} + \frac{1}{2} \Omega_{n2}^{4} \right) - \frac{1}{2} \Omega_{n2}^{6} Z \left( \Omega_{n2} \right) \right. \\ \left. + \frac{1}{2\sqrt{\pi}} \left( \Omega_{n2}^{4} + \Omega_{n2}^{2} + 2 \right) + \frac{1}{2\sqrt{\pi}} e^{-\Omega_{n2}^{2}} \left( i\pi - \text{Ei}(\Omega_{n2}^{2}) + \frac{1}{2} \ln(\Omega_{n2}^{2}) - \frac{1}{2} \ln(\Omega_{n2}^{-2}) - 2 \ln(\Omega_{n2}) \right) \right].$$
(44)



#### MISK used to compare numerical/ analytical solution of I<sub>e</sub> for ITER case: compares well\*



- Reasonable agreement gives confidence that MISK is properly computing the energy integral
  - Useful when comparing to other codes
  - Similar calculation made for both Solov'ev 1 and 3 cases using MISK
    - Also found that numerical computation compares well to analytical
  - \*Note: calculation for trapped thermal ions

## Convergence study vs. damping parameter shows no issues with zero damping



FIG. 24. Convergence of  $\delta W_K$  versus damping for the Solov'ev 1 case, as calculated by a) MARS-K, and b) MISK. For MISK, blue indicates numerical evaluation of the energy integral and black indicates analytical.

- Damping from either collisions or mode growth rate.
- Both codes converge, but to different values.

#### Kruskal-Oberman limit calculations performed: MISK and MARS-K results differ by 50% (should be closer)

In the Kruskal-Oberman limit  $|\omega_E - \omega| \to \infty$  and therefore

$$I_{\varepsilon}\left(\Psi,\Lambda,l\right)\to I_{\varepsilon}^{KO}=\int_{0}^{\infty}\hat{\varepsilon}^{\frac{5}{2}}e^{-\hat{\varepsilon}}d\hat{\varepsilon}=\frac{15\sqrt{\pi}}{8}.$$

In this limit  $\delta W_K$  is purely real, and independent of the mode-particle resonances. This allows a good check on the  $|\langle H/\hat{\varepsilon} \rangle|^2$  part of the problem.

 $\delta W_{\rm K}/-\delta W_{\rm m}$  for MISK (blue) and MARS-K (red)  $\sqrt{}$ 

						<b>\</b>		
	thermal ions			$\operatorname{the}$				
	trapped		circulating	$\operatorname{trap}$	ped	circulating	Total	
	l = 0	$l \neq 0$	enequating	l = 0	$l \neq 0$	chredhating		
Q_l1						(	$1.57 \times 10^{-1}$	
Solov ev 1	$1.11\times 10^{-2}$	$1.02\times 10^{-2}$	$9.69\times 10^{-2}$	$1.11\times 10^{-2}$	$1.02\times 10^{-2}$	$9.69\times10^{-2}$	$2.36 \times 10^{-1}$	
Solow'ou 2								
2010/ 6/ 2	$1.16\times10^{-1}$	$4.84\times10^{-2}$	$1.80\times10^{-1}$	$1.16\times 10^{-1}$	$4.84\times10^{-2}$	$1.80\times10^{-1}$	$6.89 \times 10^{-1}$	
ITED								
TTER	$5.83\times10^{-1}$	$5.20\times10^{-1}$	2.74	$7.02\times10^{-1}$	$6.01\times10^{-1}$	3.30	8.46	

- Major simplification ( $I_{\epsilon}$  = constant) gives key clue to issue
  - Different indicates the issue is in the perturbed Lagrangian.
  - Solution to differences in Lagrangian may eliminate most of the problem.

#### MARS-K and MISK energy integrals now agree\* for Solov'ev 1 equilibrium



- Attaining agreement
  - Required properly matching frequency inputs
  - Flip sign of imaginary part
  - Positive I in MISK is negative in MARS-K
    - Because of MARS-K lefthanded coordinate system?
  - \*Note: calculation for trapped thermal ions
    - Expand to all particles

#### XXX



### MARS-K adopts an MHD – drift kinetic hybrid formulation for both thermal & hot particles



#### HAGIS Suite of codes (+references) - Stability



**()** NSTX-U

## Started code comparison with simple equilibria and profile assumptions



$$\mu_0 P(\psi) = -\frac{1+\kappa^2}{\kappa R_0^3 q_0} \psi, \quad F(\psi) = 1$$
$$\psi = \frac{\kappa}{2R_0^3 q_0} \left[ \frac{R^2 Z^2}{\kappa^2} + \frac{1}{4} \left( R^2 - R_0^2 \right)^2 - a^2 R_0^2 \right]$$
$$\delta W_K \propto \int \left[ \frac{\omega_{*N} + \left(\hat{\varepsilon} - \frac{3}{2}\right) \omega_{*T} + \omega_E}{\langle \omega_D \rangle + l\omega_b + \omega_E} \right] \hat{\varepsilon}^{\frac{5}{2}} e^{-\hat{\varepsilon}} d\hat{\varepsilon}$$

- Common ground for codes (MARS / HAGIS / MISK)
  - Solov'ev equilibria
  - Codes run in perturbative mode
  - Density gradient
     constant
  - No energetic particles
  - $-\omega_r, \gamma, \nu_{eff} = 0$

Simplified resonant denominator due to assumptions

#### **Expanded comparison to include ITER equilibrium**



- More realistic case (ITER)
  - ITPA MHD WG7 equilibrium
    - $I_p = 9 \text{ MA}, \beta_N = 2.9 \text{ (7\% above } n = 1 \text{ no-wall limit)}$
  - Codes run in perturbative mode
  - With/without energetic particles

$$-\omega_{\rm r}, \gamma, \nu_{\rm eff} = 0$$

$$\delta W_K \propto \int \left[ \frac{\omega_{*N} + \left(\hat{\varepsilon} - \frac{3}{2}\right)\omega_{*T} + \omega_E}{\langle \omega_D \rangle + l\omega_b + \omega_E} \right] \hat{\varepsilon}^{\frac{5}{2}} e^{-\hat{\varepsilon}} d\hat{\varepsilon}$$

<u>Note</u>: Simplified resonant denominator due to assumptions

### Shaped vs. near-circular Solov'ev cases have important q profile differences for benchmarking



Differences in how MARS, MISK, HAGIS consider mode dissipation at rational surfaces is thought to be key – will be a main focus of next steps

#### The kinetic term can be split into two pieces that depend on the eigenfunction or the frequencies, for code comparison



# Eigenfunction benchmarking calculations were made to yield similar eigenfunctions, which are verified



- PEST, MARS-K compared with-wall RWM
  - In PEST we use the wall position that yields marginal stability
  - PEST, MARS-K, and MISHKA compared for no-wall ideal kink
- There are some differences at rational surfaces
  - May lead to stability differences between MISK and MARS-K calculations

## Bounce frequency vs. pitch angle compares well between codes



here,  $\epsilon_r$  is the inverse aspect ratio, s is the magnetic shear, K and E are the complete elliptic integrals of the first and second kind, and  $\Lambda = \mu B_0/\epsilon$ , where  $\mu$  is the magnetic moment and  $\epsilon$  is the kinetic energy.

### Bounce and precession drift frequency radial profiles agree (deeply trapped regime shown)



$$\frac{\omega_b}{\sqrt{2\varepsilon/m_i}} = \frac{1}{q_0} \left(\frac{F^2}{1+2\epsilon_r} + \frac{\kappa^2 \epsilon_r^2}{q_0^2}\right)^{-1} \left[\frac{F^2 \epsilon_r}{2\left(1+2\epsilon_r\right)} + \frac{\kappa^2 \epsilon_r^3}{q_0^2} + \frac{\left(1-\kappa^2\right) \epsilon_r^2}{2q_0^2}\left(1+2\epsilon_r\right)\right]^{\frac{1}{2}}$$

Good agreement across entire radial profile

### Significant issue found: precession drift frequencies did not

agree



- Clear difference in drift reversal point, even in near-circular case
- Issue found and corrected: metric coefficients for non-orthogonal grid incorrect in PEST interface to MISK

$$\frac{|\text{arge aspect ratio approximation}}{\langle \omega_D \rangle} = \frac{2q\Lambda}{R_0^2 B_0 \epsilon_r} \begin{bmatrix} (2s+1) \frac{E(k^2)}{K(k^2)} + 2s(k^2-1) - \frac{1}{2} \end{bmatrix} \qquad k = \begin{bmatrix} \frac{1-\Lambda + \epsilon_r \Lambda}{2\epsilon_r \Lambda} \end{bmatrix}^{\frac{1}{2}} \qquad \text{[Jucker et al., Phys. Plasmas 15, 112503 (2008)]} \end{bmatrix}$$

(2008)]



• Metric coefficients corrected in PEST interface to MISK

$$\omega_D = -\frac{1}{\tau} \int \frac{1}{v_{\parallel}} \mathbf{v}_{\mathbf{D}} \cdot \left( \boldsymbol{\nabla}\phi - \hat{q} \boldsymbol{\nabla}\theta \right) d\boldsymbol{\ell} - \frac{1}{\tau} \int_{\boldsymbol{\theta}(t)}^{\boldsymbol{\theta}(t')} \hat{q} d\theta$$

if  $\Psi$  and  $\theta$  are orthogonal:

$$\hat{q}\mathbf{B} \times \boldsymbol{\nabla}\theta = \frac{\left(\mathbf{B}_{\phi} \cdot \boldsymbol{\nabla}\phi\right)\left(\mathbf{B}_{\phi} \times \boldsymbol{\nabla}\theta\right)}{\mathbf{B}_{\theta} \cdot \boldsymbol{\nabla}\theta}$$

But in PEST,  $\Psi$  and  $\theta$  are non-orthogonal:

$$\hat{q}\mathbf{B} \times \boldsymbol{\nabla}\boldsymbol{\theta} = \underbrace{\mathbf{B}_{\phi} \cdot \boldsymbol{\nabla}\phi}_{\left(\mathbf{B}_{\phi} \cdot \boldsymbol{\nabla}\boldsymbol{\theta}\right) + \mathbf{B}_{\theta} \cdot \boldsymbol{\nabla}\boldsymbol{\theta}}_{\left(\mathbf{B}_{\phi} \times \boldsymbol{\nabla}\boldsymbol{\theta} + \mathbf{B}_{\theta} \times \boldsymbol{\nabla}\boldsymbol{\theta}\right)} \left(\mathbf{B}_{\phi} \times \boldsymbol{\nabla}\boldsymbol{\theta} + \mathbf{B}_{\theta} \times \boldsymbol{\nabla}\boldsymbol{\theta}\right)$$

### <u>How does $\omega_D$ correction effect NSTX results</u>? Mostly affects outer

surfaces; characteristic change of  $\gamma \tau_w$  with  $\omega_{\phi}$  is the same.



<u>RWM stability vs.  $ω_{\phi}$  (contours of  $\gamma \tau_{w}$ )</u>



- Affects magnitude of δW<sub>κ</sub>, but not trends
- In this case, agreement with the experimental
  - marginal point improves
    Calculations continue to
    - Calculations continue to determine the effect of the correction on wider range of cases

