The Method of Harmonic Balance for Differential Constitutive Models in Oscillatory Shear

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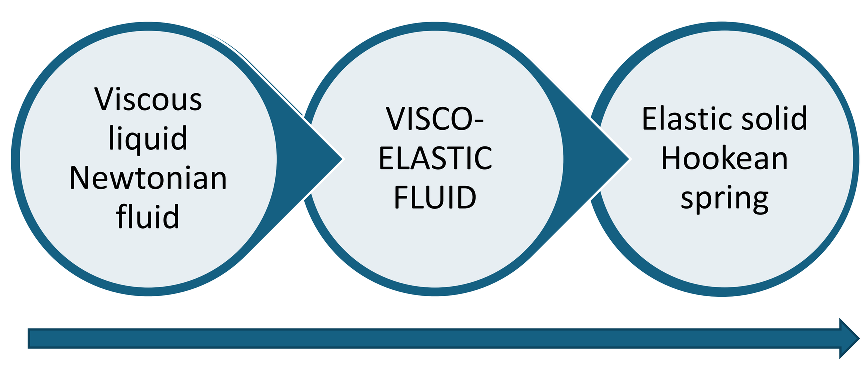
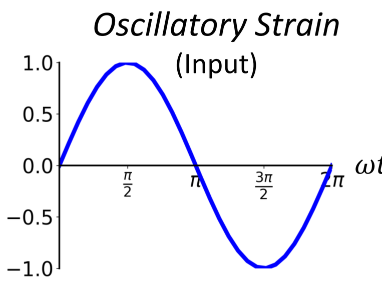
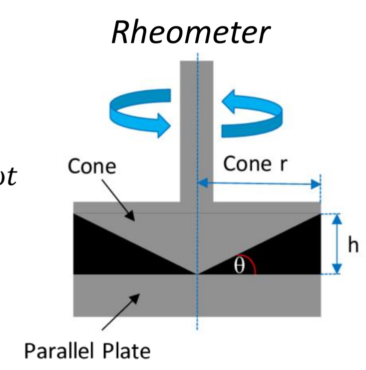
Oscillatory Shear Rheology

Mechanical response to an applied shear deformation

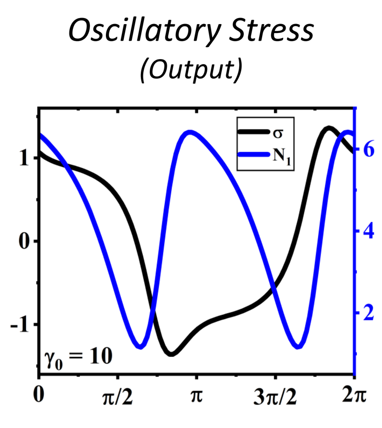




$\gamma(t) = \gamma_0 \sin \omega t$



Dynamic Oscillatory Shear tests are used to probe viscoelasticity



Shear Stress

$$\sigma = \gamma_0 \sum_{n=1,\text{odd}}^{\infty} G_n' \sin(n\omega t) + G_n'' \cos(n\omega t)$$

Fourier Series

First Normal Stress difference

$$N_1 = \gamma_0^2 \sum_{n=0,\text{even}}^{\infty} F_n' \sin(n\omega t) + F_n'' \cos(n\omega t)$$

The component of $\sigma(t)$ in-phase (out of phase) with $\gamma(t)$ describes the elastic (viscous) nature of the material

Constitutive Models

A constitutive model (CM) is a set of mathematical equations that describe the relation between the extra stress tensor $\boldsymbol{\sigma}$ and strain γ.

- Physical interpretation of experimental data through Fourier coefficients is not straightforward
- There is a need to use Constitutive theories for OS analysis
- Analytical OS solutions are not available for a majority of nonlinear differential CMs.
- The conventional approach of using numerical integration (NI) is slow.

We propose the use of a fast and spectrally accurate method to solve nonlinear CMs under OS flow called ***Harmonic balance***

Corotational Maxwell model (CMM)

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{\Omega}\cdot\boldsymbol{\sigma} - \boldsymbol{\sigma}\cdot\boldsymbol{\Omega}) + \frac{\boldsymbol{\sigma}}{\lambda} = G\dot{\boldsymbol{\gamma}}$$

$$\boldsymbol{\Omega} = \frac{1}{2}(\nabla \mathbf{v} - \nabla \mathbf{v}^T)$$

Giesekus model

$$\overset{\triangledown}{\boldsymbol{\sigma}} + \frac{\boldsymbol{\sigma}}{\lambda} + \frac{\alpha}{\lambda G}\boldsymbol{\sigma}\cdot\boldsymbol{\sigma} = G\dot{\boldsymbol{\gamma}}$$

PTT model

$$\overset{\triangledown}{\boldsymbol{\sigma}} + g(\boldsymbol{\sigma})\frac{\boldsymbol{\sigma}}{\lambda} = G\dot{\boldsymbol{\gamma}}$$

$$g(\boldsymbol{\sigma}) = \exp(\varepsilon\, \mathrm{tr}(\boldsymbol{\sigma}))$$

Temporary Network model (TNM)

$$\overset{\triangledown}{\boldsymbol{\sigma}} + d(t)\frac{\boldsymbol{\sigma}}{\lambda} - \frac{G}{\lambda}(c(t) - d(t)) = G\dot{\boldsymbol{\gamma}}$$

$$c(t) = \exp(a|\sigma_{12}|)$$

$$d(t) = \exp(b|\sigma_{12}|)$$

$$\overset{\triangledown}{\boldsymbol{\sigma}} = \frac{\partial \boldsymbol{\sigma}}{\partial t} - \boldsymbol{\sigma}\cdot\nabla\mathbf{v} - \nabla\mathbf{v}^T\cdot\boldsymbol{\sigma}$$

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{12} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}$$

$$\dot{\boldsymbol{\gamma}} = \frac{1}{2}\gamma_0\omega\cos\omega t \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Harmonic Balance

Harmonic balance (HB) is used for nonlinear vibration problems where long-time the response to an oscillatory input is also oscillatory or a periodic steady state .

System of nonlinear ODEs in the time domain

$$\boldsymbol{r} = \dot{\boldsymbol{q}} + \boldsymbol{f}_{nl}(\boldsymbol{q}, t) - \boldsymbol{f}_{ex}(t) = \boldsymbol{0}$$

Fourier Series

$$q_i(t) \approx q_i^H(t) = \hat{\boldsymbol{q}}_i \cdot \boldsymbol{B}^H$$

$$\boldsymbol{r}^H = \dot{\boldsymbol{q}}^H + \boldsymbol{f}_{nl}(\boldsymbol{q}^H, t) - \boldsymbol{f}_{ex}(t) = \boldsymbol{0}$$

Fourier Transform

$$\boldsymbol{r}^H = \hat{\boldsymbol{r}}^H \cdot \boldsymbol{B}^H = 0$$

Frequency domain residual

$$\hat{\boldsymbol{r}}^H = \hat{\dot{\boldsymbol{q}}}^H + \hat{\boldsymbol{f}}_{nl}(\hat{\boldsymbol{q}}^H) - \hat{\boldsymbol{f}}_{ex} = \boldsymbol{0}$$

System of nonlinear algebraic equations in the frequency domain

$$q_i^H(t) = \hat{q}_i(0) + \sum_{k=1}^{H}\begin{pmatrix}\hat{q}_{c,i}(k)\cos k\omega t \\ +\hat{q}_{s,i}(k)\sin k\omega t\end{pmatrix}$$

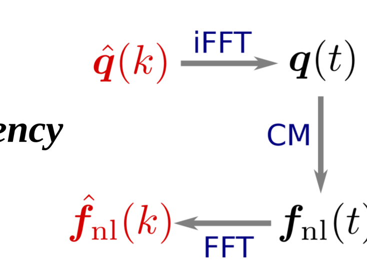
OR

$$q_i^H(t) = \sum_{k=-H}^{H} \hat{q}_i(k) e^{ik\omega t}$$

Symbol	Description
De = λω	Deborah number
Wi = λωγ₀	Weissenberg number
$\boldsymbol{r}$	Residual term
$\boldsymbol{q}$	Unknown variables
$\boldsymbol{B}$	Set of basis functions (Sine-cosine or exponential)
H	No. of harmonics
$\hat{\boldsymbol{r}}, \hat{\boldsymbol{q}}$	Set of Fourier coefficient of r and q

For many systems (PTT and TNM) direct transformation of the time domain ODEs to the frequency domain is not possible. We use an alternate mechanism

Alternating Frequency Time (AFT)



The AFT scheme can be used to implement HB on any differential constitutive model with any nonlinearity

HB for CMM

The CMM has an analytical solution (AS) reported in the literature. The solution is an infinite Fourier series containing Bessel functions. We compare this AS with the HB solution.

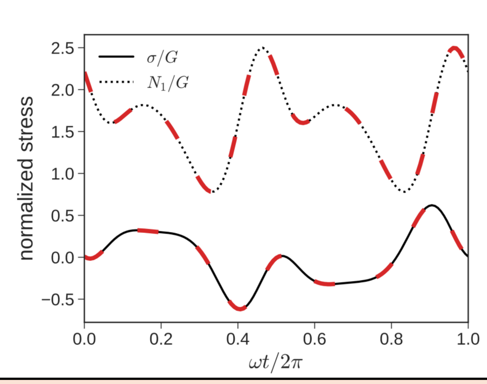
Exponential Fourier series

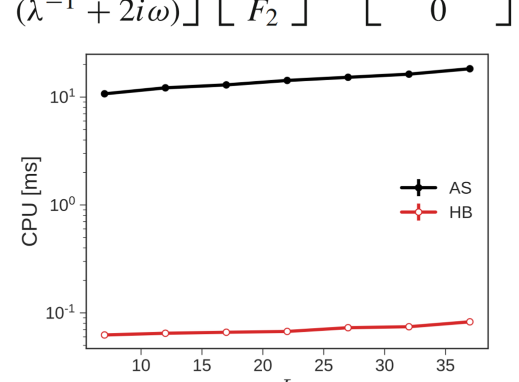
$$\sigma_{12} = \sum_{k=-(H-1)}^{H} S_{2k+1} e^{i(2k+1)\omega t}$$

$$N_1 = \sigma_{11} - \sigma_{22} = \sum_{k=-H}^{H} F_{2k} e^{i2k\omega t}$$

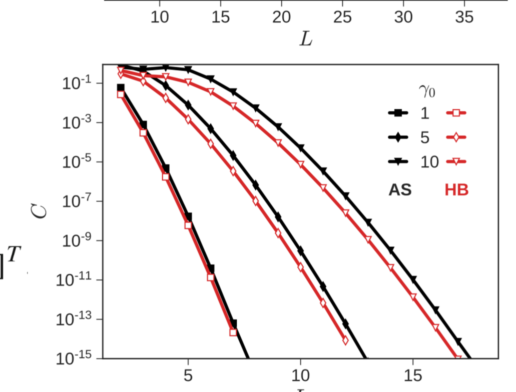
HB leads to a tridiagonal linear system. For $H = 1$

$$\begin{bmatrix} (\lambda^{-1} - 2i\omega) & -\gamma_0\omega & 0 & 0 & 0 \\ \gamma_0\omega/4 & (\lambda^{-1} - i\omega) & \gamma_0\omega/4 & 0 & 0 \\ 0 & -\gamma_0\omega & \lambda^{-1} & -\gamma_0\omega & 0 \\ 0 & 0 & \gamma_0\omega/4 & (\lambda^{-1} + i\omega) & \gamma_0\omega/4 \\ 0 & 0 & 0 & -\gamma_0\omega & (\lambda^{-1} + 2i\omega) \end{bmatrix} \begin{bmatrix} F_{-2} \\ S_{-1} \\ F_0 \\ S_1 \\ F_2 \end{bmatrix} = \begin{bmatrix} 0 \\ G\gamma_0\omega/2 \\ 0 \\ G\gamma_0\omega/2 \\ 0 \end{bmatrix}$$





HB solution agrees well with the AS and has a comparable convergence rate but, it is much faster. =



$$X = [N_1(t_1), \cdots, N_1(t_{N_t}), \sigma(t_1), \cdots, \sigma(t_{N_t})]^T$$

$$C(L) = \|\Delta X(L)\| / \|X(L)\|$$

HB for Giesekus Model

$$\boldsymbol{q} = [\sigma_{11}\ \sigma_{22}\ \sigma_{12}]^T$$

External forcing function

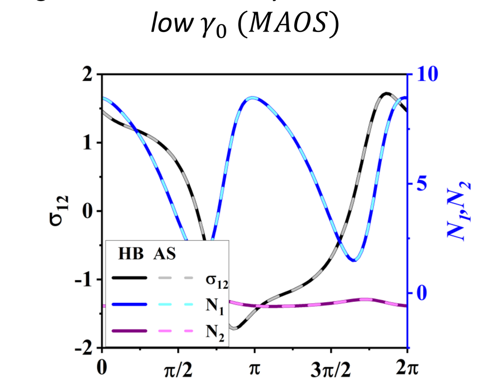
$$\boldsymbol{f}_{ex} = [0\ 0\ 0\ G\gamma_0\omega\cos\omega t]^T$$

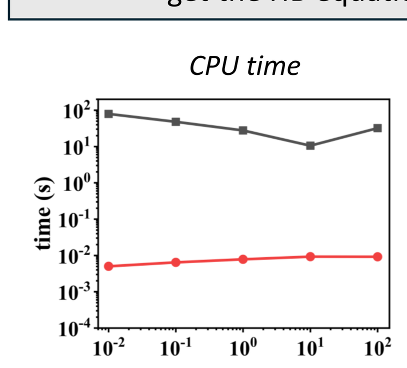
Nonlinear terms

$$\boldsymbol{f}_{nl} = \begin{bmatrix} \frac{\sigma_{11}}{\lambda} + \frac{\alpha}{\lambda G}(\sigma_{11}^2 + \sigma_{12}^2) - 2\dot{\gamma}\sigma_{12} \\ \frac{\sigma_{22}}{\lambda} + \frac{\alpha}{\lambda G}(\sigma_{22}^2 + \sigma_{12}^2) \\ \frac{\sigma_{12}}{\lambda} + \frac{\alpha}{\lambda G}\sigma_{12}(\sigma_{11} + \sigma_{22}) - \dot{\gamma}\sigma_{22} \end{bmatrix}$$

Take Fourier transform of each of the terms to get the HB equation system

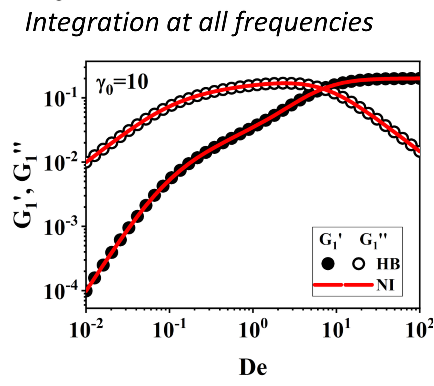
Agreement with analytical solution at low γ_0 (MAOS)

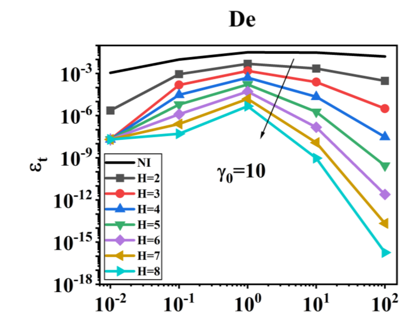




HB solution agrees well with Ni and AS and is faster, more accurate, and shows exponential convergence.

Agreement with Numerical Integration at all frequencies





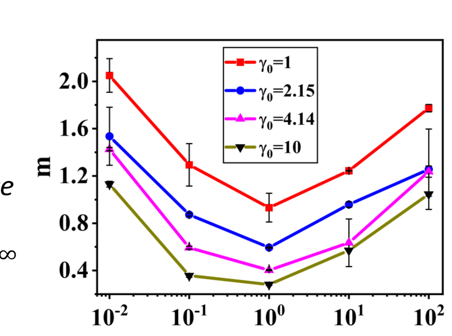
Time domain residual

$$\varepsilon_t \propto \left\| r(q^H) \right\|_2$$

Exponential Convergence

$$\|\sigma\|_\infty = \left\| \sigma_{12}^{HB} - \sigma_{12}^{AS} \right\|_\infty$$

$$\|\sigma\|_\infty \propto e^{-m(2H-1)}$$



HB for Other Nonlinear CMs

To implement HB on other nonlinear differential CMs, a HB+AFT scheme is used. By simply changing the nonlinear term $\boldsymbol{f}_{nl}$ we can get oscillatory shear responses of any CM. We define a general form for any nonlinear CM

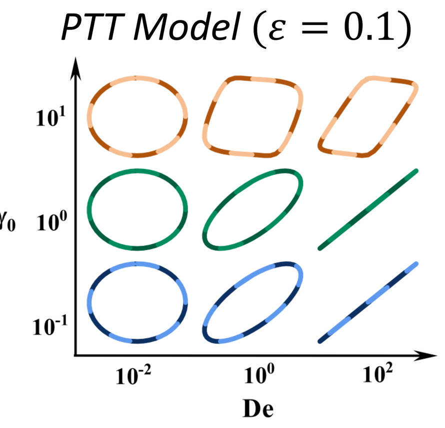
$$\overset{\triangledown}{\boldsymbol{\sigma}} + \zeta\left(\boldsymbol{\gamma}_{(1)}\cdot\boldsymbol{\sigma} + \boldsymbol{\sigma}\cdot\boldsymbol{\gamma}_{(1)}\right) + \frac{1}{\lambda}\boldsymbol{H}(\boldsymbol{\sigma}) + \boldsymbol{J}(\boldsymbol{\sigma}) - (1-\zeta)G\boldsymbol{\gamma}_{(1)} = 0$$

$$\boldsymbol{f}_{nl} = \begin{bmatrix} 2\zeta\sigma_{12}\dot{\gamma} + \frac{1}{\lambda}H_{11}(\boldsymbol{\sigma}) + J_{11}(\boldsymbol{\sigma}) \\ 2\zeta\sigma_{12}\dot{\gamma} + \frac{1}{\lambda}H_{22}(\boldsymbol{\sigma}) + J_{22}(\boldsymbol{\sigma}) \\ \frac{1}{\lambda}H_{33}(\boldsymbol{\sigma}) + J_{33}(\boldsymbol{\sigma}) \\ \zeta\dot{\gamma}(\sigma_{11} + \sigma_{22}) + \frac{1}{\lambda}H_{12}(\boldsymbol{\sigma}) + J_{12}(\boldsymbol{\sigma}) + G\zeta\dot{\gamma} \end{bmatrix}$$

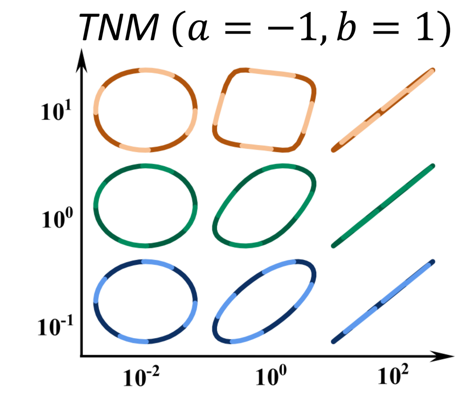
PTT	$\zeta = 0, H(\sigma) = \exp(\varepsilon\,\mathrm{tr}(\sigma))\sigma$, $J(\sigma) = 0$
TNM	$\zeta = 0, H(\sigma) = d(t)\sigma$, $J(\sigma) = -(c(t) - d(t))$, $c(t) = e^{a\lvert\sigma_{12}\rvert}, d(t) = e^{b\lvert\sigma_{12}\rvert}$

$\boldsymbol{\sigma_{12}}$ **vs** $\boldsymbol{\gamma}$ HB and NI solutions at different γ_0 and De agree well

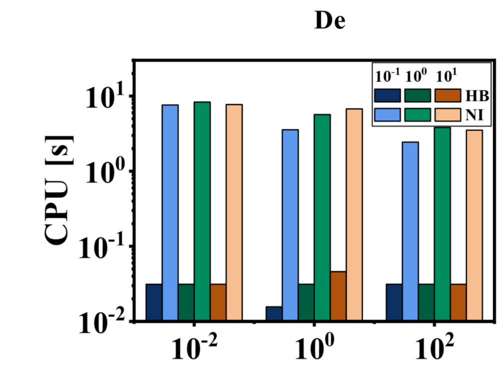
PTT Model $(\varepsilon = 0.1)$

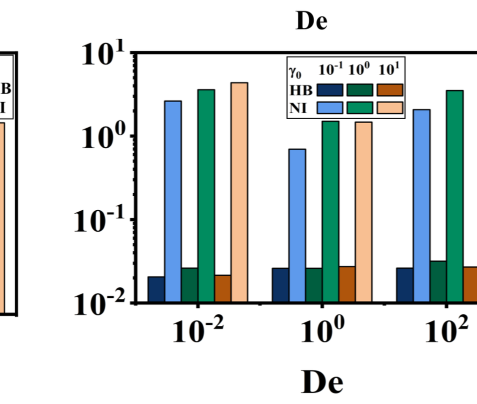


TNM $(a = -1, b = 1)$



CPU time HB is 1.5-2.5 orders of magnitude faster than NI





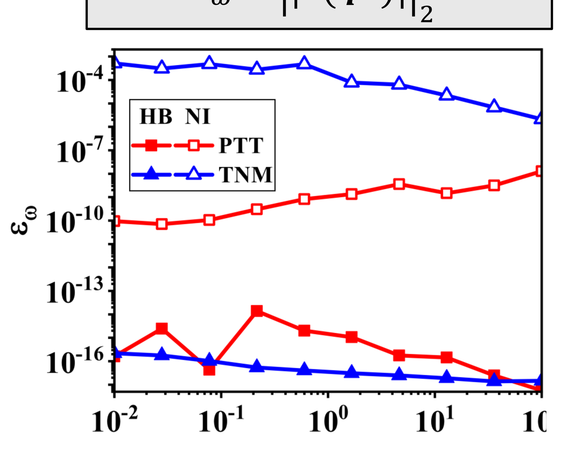
Accuracy and Convergence

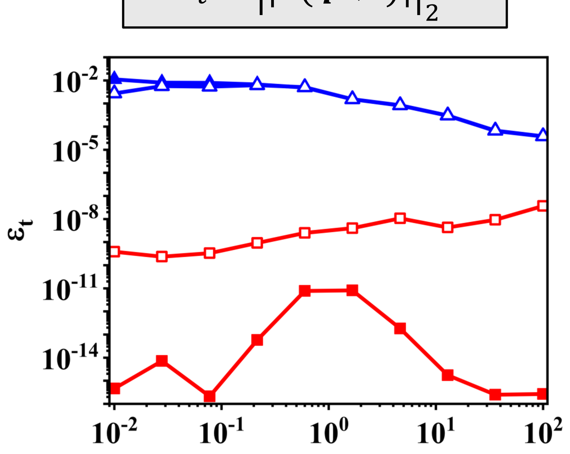
Frequency Domain Residual

$$\varepsilon_\omega \propto \left\| \hat{r}(\hat{q}^H) \right\|_2$$

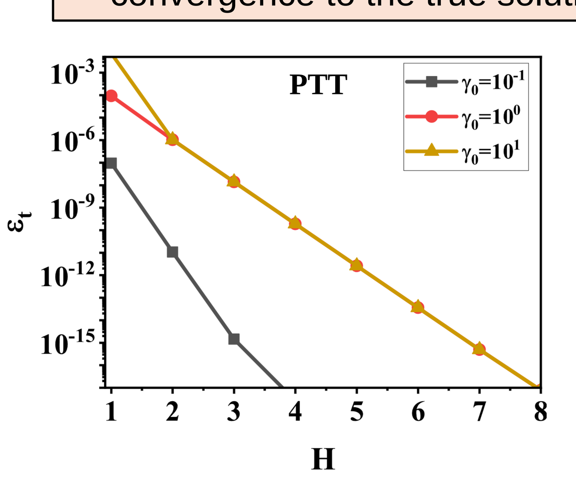
Time Domain Residual

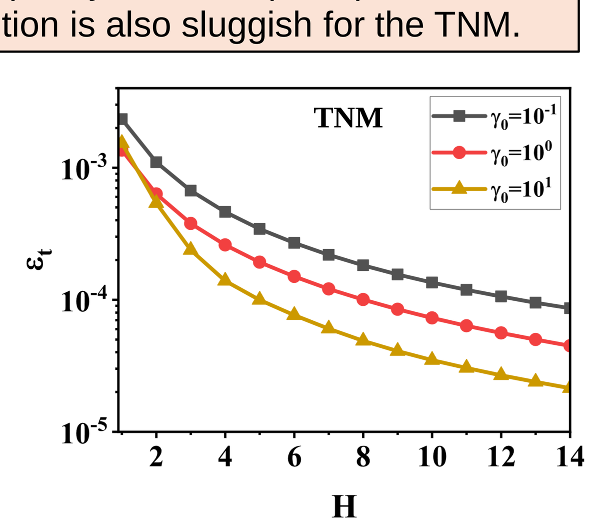
$$\varepsilon_t \propto \left\| r(q^H, t) \right\|_2$$





HB outperforms NI for the PTT model. However, both HB and Ni struggle with the TNM due to presence of non-analytic terms (c, d) as Fourier series perform poorly near sharp cusps. The convergence to the true solution is also sluggish for the TNM.



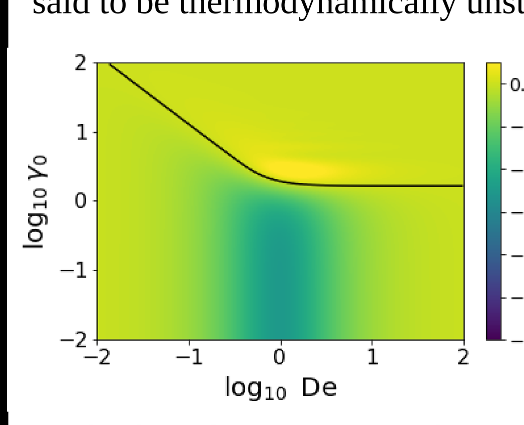


Further Theoretical Studies

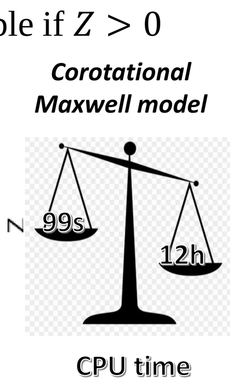
Thermodynamic Study

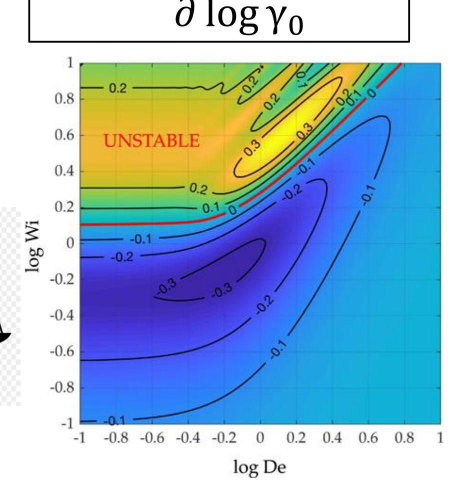
As per the Ziegler criterion proposed by Saengow and Giacomin, a system subjected to OS flow is said to be thermodynamically unstable if $Z > 0$

$$Z = -\frac{\partial \log G_1''}{\partial \log \gamma_0} - 1$$



Plot obtained using Harmonic Balance



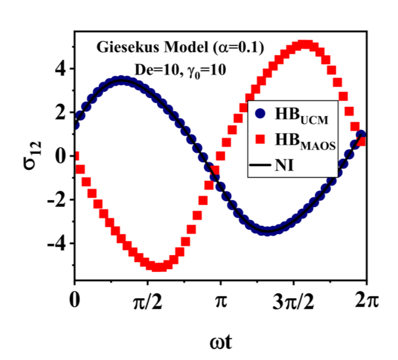


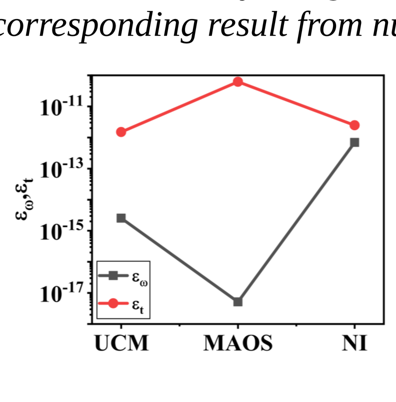
Plot given by Saengow and Giacomin using analytical solution

Such theoretical studies can be carried out on any nonlinear constitutive model with/without an analytical solution at a much lower CPU cost.

Mathematical Instabillity

HB implemented on the Giesekus model by using two different initial conditions. It is compared with the corresponding result from numerical integration.





HB facilitates study of mathematically unstable solutions by simply tweaking the initial guess values to the HB algorithm. This is not possible with NI.

Summary and Conclusions

- ✓ Harmonic Balance converts the time domain initial value problem to a frequency domain optimization problem
- ✓ For linear CMs such as the Corotational maxwell model, the HB formulation leads to a linear system of equations. HB solution turns out to be more efficient than the available analytical solution
- ✓ For CMs with polynomial terms such as the Giesekus model $(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma})$, a system of algebraic equations is obtained which can be solved with any standard nonlinear solver
- ✓ For all other CMs with arbitrary nonlinearity, the AFT scheme is coupled to the nonlinear solver that oscillates back and forth in time and frequency domain to map the nonlinear terms
- ✓ HB outperforms NI both in terms of CPU time and accuracy
- ✓ HB facilitates further theoretical studies on constitutive models subjected to LAOS flows

Publications

- Harmonic Balance for Differential Constitutive Models under Oscillatory Shear. *arXiv preprint arXiv:2403.05971* (2024)
- Can numerical methods compete with analytical solutions of linear constitutive models for large amplitude oscillatory shear flow?. *Rheologica Acta*, *63*(2), pp.145-155 (2024)
- The method of harmonic balance for the Giesekus model under oscillatory shear. *Journal of Non-Newtonian Fluid Mechanics*, *321*, p.105092 (2023)

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