Thursday 10:20 Johann-Peter-Hebel FM3

PGD-based parametric solutions of double-scale Fokker-Planck equations: application to suspensions involving aggregates of rods

Francisco Chinesta*[1], Emmanuelle Abisset-Chavanne[1], Amine Ammar[2], Marta Perez[1], Roland Keunings[3]
Francisco.Chinesta@ec-nantes.fr
[1]Ecole Centrale de Nantes, GeM, Nantes, France, [2]ENSAM Angers, LAMPA, Angers, France, [3]Universite Catholique de Louvain, CESAME, Louvain, Belgium

When suspensions composed of rods become concentrated enough rods aggregate to create clusters. These clusters can interact when the clusters concentration is large enough, or not when it remains small enough. The kinetic theory modeling of such systems requires a double scale description; the fine scale related to the rods orientation distribution existing in each cluster, and the coarse one related to clusters distribution itself. In the coarse scale the distribution depends on the second and fourth order moments of the orientation distribution of rods composing the clusters. The resulting Fokker-Planck equation involves the physical coordinates, the time and a number of conformational coordinates. Moreover it involves some material parameters related to the configuration relaxation time and the cluster's softness, as well as other parameters related to the enforced flow: shear and elongation rates. In order to analyze the influence of each material or flow parameter on the distribution function the classical route consists of performing a sampling of the parametric space and then solving the resulting multidimensional Fokker-Planck equation for each choice of those parameters. Obviously the computational complexity becomes rapidly prohibitive and then only very (too) coarse samplings of the parametric space remain affordable. PGD was proposed by the authors some years ago for addressing efficiently the solution of multidimensional Fokker-Planck equations encountered in computational rheology. Then, it was extended for addressing the solution of standard models in which parameters were considered as model extra-coordinates resulting in a parametric multidimensional equations. In this work we combine both proposals for addressing the efficient solution of parametric Fokker-Planck equations, making special attention to the advective stabilizations issues.

Thursday 11:10 Johann-Peter-Hebel FM4

Influence of channel aspect ratio on the onset of elastic instabilities in three-dimensional cross-slots

Filipe A. Cruz*[1], Robert J. Poole[2], Alexandre Afonso[1], Fernando T. Pinho[3], Paulo J. Oliveira[4], Manuel A. Alves[1]
facruz@fe.up.pt
[1]Universidade do Porto, CEFT, Departamento de Engenharia Química, Porto, Portugal, [2]University of Liverpool, School of Engineering, Liverpool, United Kingdom, [3]Universidade do Porto, CEFT, Departamento de Engenharia Mecânica, Porto, Portugal, [4]Universidade da Beira Interior, CEFT, Departamento de Engenharia Electromecânica, Covilhã, Portugal

In this work, we investigate by means of numerical simulations the existence of purely-elastic flow instabilities in three-dimensional cross-slot geometries. Specifically, we probe the effect of aspect ratio – defined as the ratio between the height and width of the rectangular cross-section of the channels – for both the upper-convected Maxwell and the Phan-Thien-Tanner constitutive models.
For both models, we observe the occurrence of a supercritical bifurcation, from a steady-state symmetric flow to an asymmetric but still steady pattern, above critical values of the Deborah number (De) and also of the aspect ratio. Further increase in De triggers a transition to time-dependent flow, a situation akin to that previously reported for two-dimensional cross-slot devices [Poole et al., Phys Rev Lett 99(16):164503, 2007].
For sufficiently low aspect ratios (shallow channels), no intermediate steady asymmetric states are observed and a direct transition to time-dependent flow occurs. Interestingly, this transition occurs at progressively lower De values when the aspect ratio of the cross-slot channel is decreased. Stability maps of aspect ratio vs. De are presented, together with a discussion on possible mechanisms for the onset of elastic instabilities.

Thursday 11:30 Johann-Peter-Hebel FM5

Non-linear dynamics of an ellipsoid in a sheared viscoelastic fluid

Gaetano D'Avino*[1], Francesco Greco[2], Martien A. Hulsen[3], Pier Luca Maffettone[1]
gadavino@unina.it
[1]Università di Napoli Federico II, Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Naples, Italy, [2]Istituto di Ricerche sulla Combustione - IRC-CNR, Naples, Italy, [3]Technische Universiteit of Eindhoven, Department of Mechanical Engineering, Eindhoven, The Netherlands

Influence of channel aspect ratio on the onset of elastic instabilities in three-dimensional cross-slots

F. A. Cruz [1,*], R. J. Poole [2], F. T. Pinho [3], P.J. Oliveira [4], M. A. Alves [1]

[1] Departamento de Engenharia Química, CEFT, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

[2] School of Engineering, University of Liverpool, Brownlow Street, Liverpool, L69 3GH United Kingdom

[3] CEFT, Departamento de Engenharia Mecânica, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

[4] Departamento de Engenharia Electromecânica, Materiais Têxteis e Papeleiros, Universidade da Beira Interior, 6201-001 Covilhã, Research Unit CEFT,Portugal

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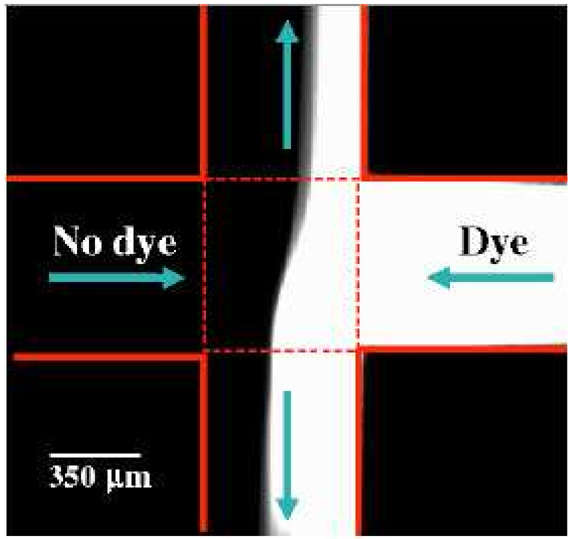
Outline

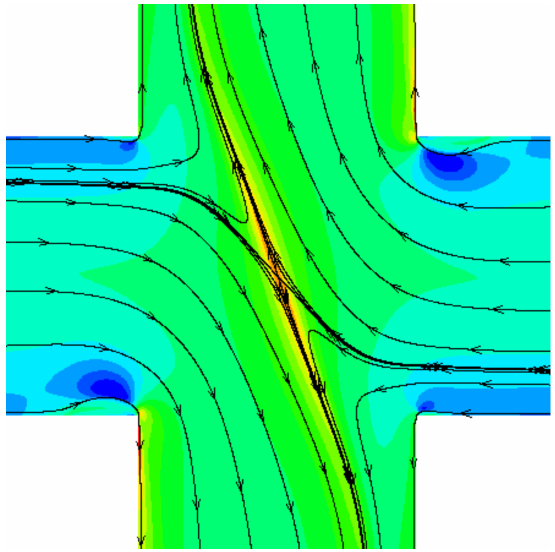
- Motivation
- Governing equations and numerical methods
- Geometry and meshes
- Data processing
- Results
  - **AR_N–De** stability diagrams for UCM and sPTT constitutive models.
  - Analysis of associated relevant parameters.

Motivation – Expanding upon previous work

- So far simulations have mostly focused on 2D geometries.
- However, experimental geometries are 3D.
- **What type of 3D effects, if any, can we expect?**



PAA solution, Re<0.01, De=4.5



sPTT model, β=1/9, ε=0.02, De=0.9

Arratia et al., Phys Rev Lett. 96 (2006) 144502.

Same year: Pathak and Hudson, Macromolecules. 39 (2006) 8782–8792.

Earlier observations: Gardner et al., Polymer. 23 (1982) 1435–1442.

Recent work: Cruz et al., A new viscoelastic benchmark flow: stationary bifurcation in a cross-slot. *Submitted manuscript.*

Motivation – Goals

- Obtain data for a wide range of aspect ratios, for different constitutive models.
  - UCM
  - sPTT, β=1/9, ε=0.02
- Study how the aspect ratio affects flow stability, specifically at the stagnation point.

Governing equations

- Inertialess $\left(Re \to 0\right)$, isothermal, incompressible flow.
  - Conservation of mass: $\nabla \cdot \mathbf{u} = 0$
  - Conservation of momentum: $-\nabla p + \nabla \cdot \boldsymbol{\tau} + \beta \eta_o \nabla^2 \mathbf{u} = \mathbf{0}$
  - Constitutive equation (sPTT model):

UCM model for β=0

$$\beta = \frac{\eta_s}{\eta_s + \eta_p}$$

$$\left(1 + \frac{\lambda \varepsilon}{\left(1-\beta\right)\eta_o} \mathrm{Tr}\left(\boldsymbol{\tau}\right)\right)\boldsymbol{\tau} + \lambda\left[\frac{\partial \boldsymbol{\tau}}{\partial t} + \nabla \cdot \mathbf{u}\boldsymbol{\tau}\right] = \left(1-\beta\right)\eta_o\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right) + \lambda\left(\boldsymbol{\tau} \cdot \nabla \mathbf{u} + \nabla \mathbf{u}^T \cdot \boldsymbol{\tau}\right)$$

UCM model for ε=0

Numerical methods

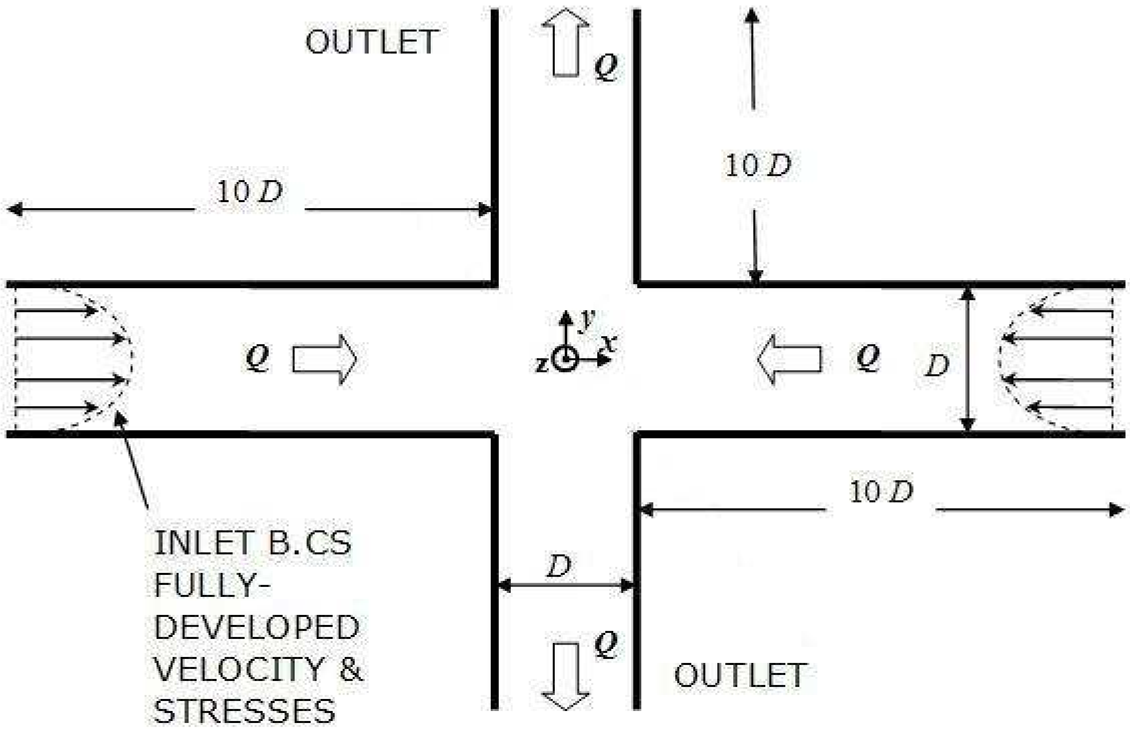
- Fully implicit finite volume method (Oliveira et al., 1998)
  - Structured, collocated and non-orthogonal meshes
  - Time-marching algorithm
  - Diffusive terms: central differences scheme (CDS)

  - Advective terms, high resolution scheme: CUBISTA (Alves et al., 2003)

  - Log-conformation technique for polymeric stress tensor (Afonso et al., 2009)

Oliveira et al., J Non-Newton Fluid. 79 (1998) 1–43.
Alves et al., Int J Numer Meth Fl. 41 (2003) 47–75.
Afonso et al., J Non-Newton Fluid. 157 (2009) 55–65.

Geometry



$$AR = \frac{H}{D}; \quad AR_N = \frac{AR}{AR+1}$$

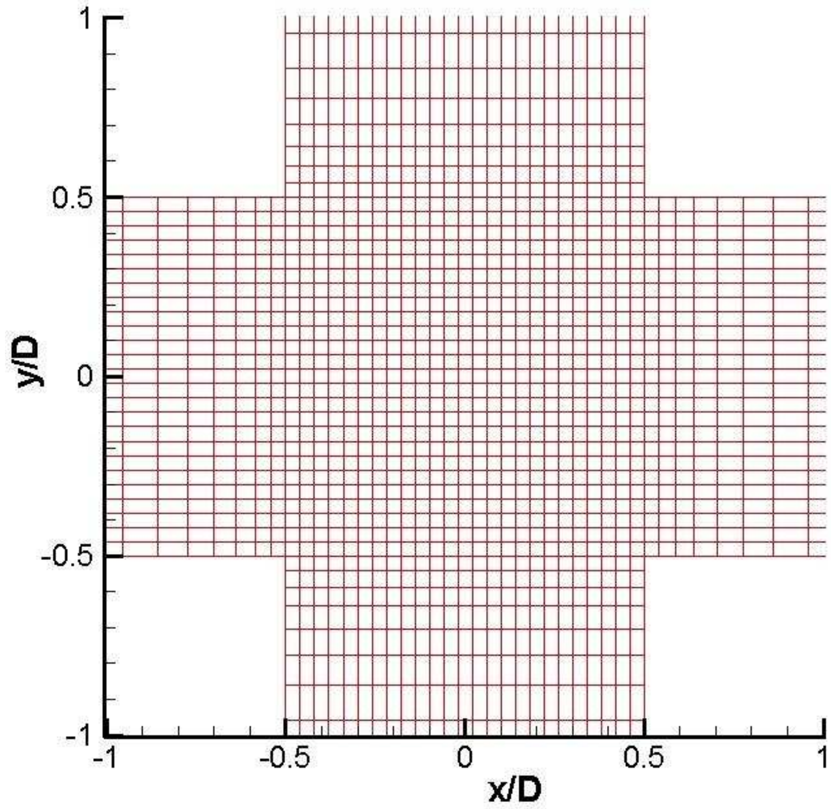
AR_N	**H/D**
0.01	0.010
0.1	0.11
0.2	0.25
0.3	0.43
0.4	0.67
0.5	1.0
0.6	1.5
0.7	2.3
0.8	4.0
0.9	9.0
1	∞

Top-Bottom symmetry boundary conditions.

3D meshes

Mesh	Configuration	NC	$\frac{\Delta x_{\min}}{D} = \frac{\Delta y_{\min}}{D}$
3D	25x25x25(x5)	78125	0.04
2D	101x101(x5)	51005	0.01

Top-down view



AR_N	H/D	Δz/D
0.01	0.010	0.00040
0.1	0.11	0.0044
0.2	0.25	0.010
0.3	0.43	0.017
0.4	0.67	0.027
0.5	1.0	0.040
0.6	1.5	0.060
0.7	2.3	0.093
0.8	4.0	0.16
0.9	9.0	0.36

Data processing

- Calculation of Wi at the stagnation point
  - Assuming a locally linear velocity field:

$$\nabla \mathbf{u} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial v}{\partial x} & \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} & \frac{\partial v}{\partial y} & \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} & \frac{\partial v}{\partial z} & \frac{\partial w}{\partial z} \end{bmatrix} \rightarrow \begin{matrix} \det\left(\nabla \mathbf{u} - \lambda \mathbf{I}\right) = 0 \\ \left(\nabla \mathbf{u}\right)\mathbf{v} = \lambda \mathbf{v} \end{matrix} \rightarrow \begin{matrix} \lambda_a \rightarrow \mathbf{a} \\ \lambda_b \rightarrow \mathbf{b} \\ \lambda_c \rightarrow \mathbf{c} \end{matrix}$$

strain-rates

principal directions of strain

e.g. Newtonian fluid:

$$\begin{aligned} \lambda_a &= \dot{\varepsilon}_x < 0 & \mathbf{a} &= \hat{\mathbf{i}} \\ \lambda_b &= \dot{\varepsilon}_y = -\dot{\varepsilon}_x & \mathbf{b} &= \hat{\mathbf{j}} \\ \lambda_c &= \dot{\varepsilon}_z = 0 & \mathbf{c} &= \hat{\mathbf{k}} \end{aligned}$$

Data processing

- Calculation of Wi at the stagnation point
  - Conservation of mass: $\Rightarrow \dot{\varepsilon}_a + \dot{\varepsilon}_b + \dot{\varepsilon}_c = 0$

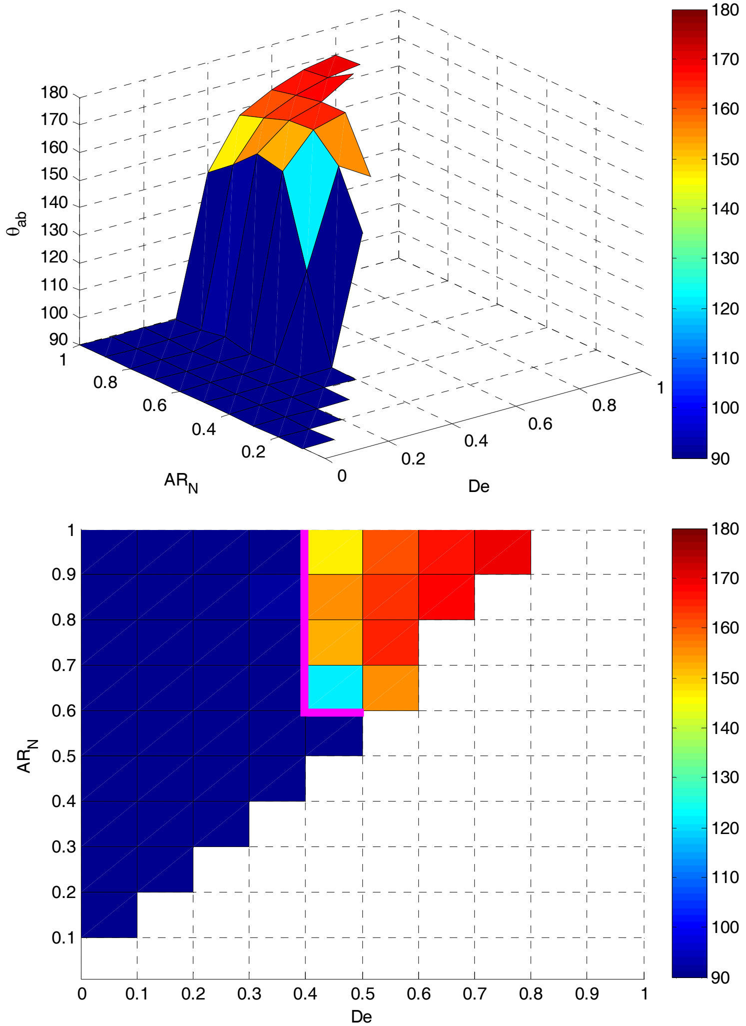
$$\Rightarrow \left|\dot{\varepsilon}_a\right| = \left|\dot{\varepsilon}_b\right| + \left|\dot{\varepsilon}_c\right|$$
$$\vee \left|\dot{\varepsilon}_b\right| = \left|\dot{\varepsilon}_a\right| + \left|\dot{\varepsilon}_c\right|$$
$$\vee \left|\dot{\varepsilon}_c\right| = \left|\dot{\varepsilon}_a\right| + \left|\dot{\varepsilon}_b\right|$$

$$\Rightarrow Wi_0 = \lambda \times \max\left(\left|\dot{\varepsilon}_a\right|, \left|\dot{\varepsilon}_b\right|, \left|\dot{\varepsilon}_c\right|\right)$$

- Asymmetry parameter
  - if then $\mathbf{c} \| \hat{\mathbf{k}}$ $\mathbf{a} \angle \mathbf{b}$

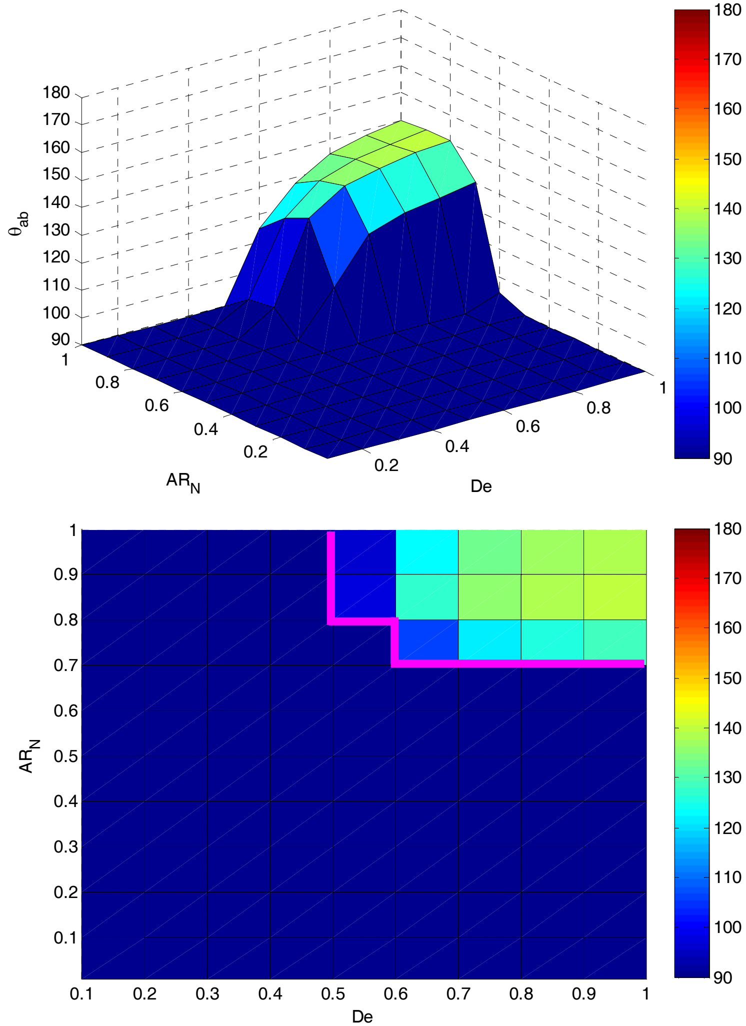
Stability diagrams – Degree of asymmetry

UCM model



UCM: Potential for unbounded stresses above Wi>0.5.

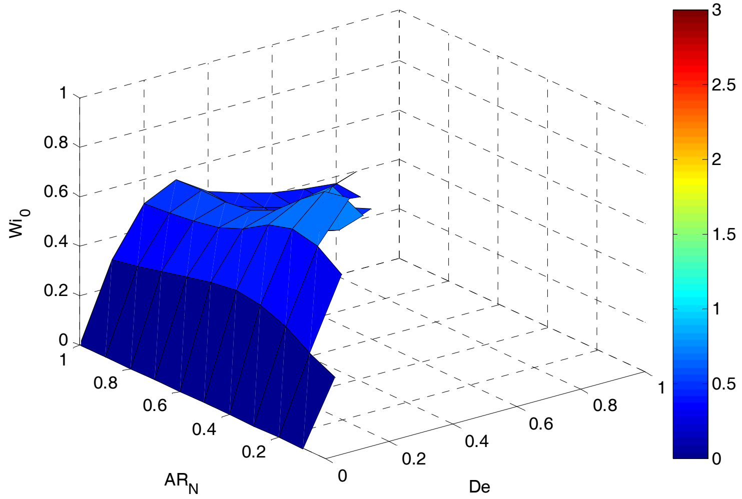
sPTT model, β=1/9, ε=0.02

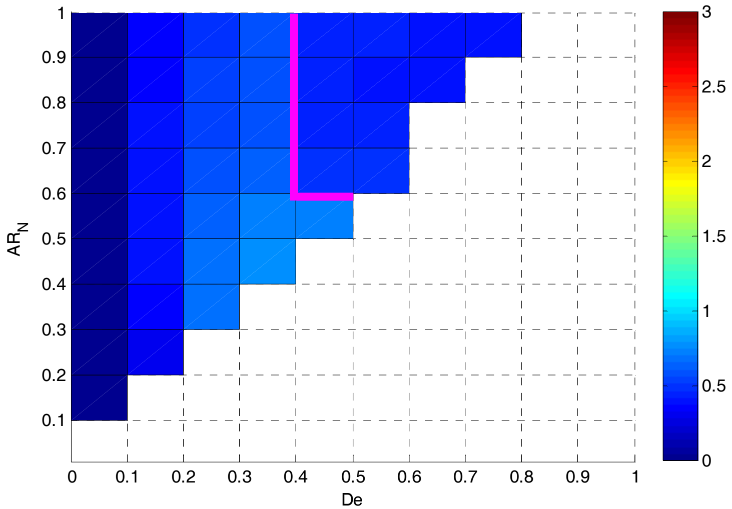


PTT: Shear-thinning; effective λ, and thus Wi, is lower than imposed λ.

Stability diagrams – Weissenberg at stagnation point

UCM model





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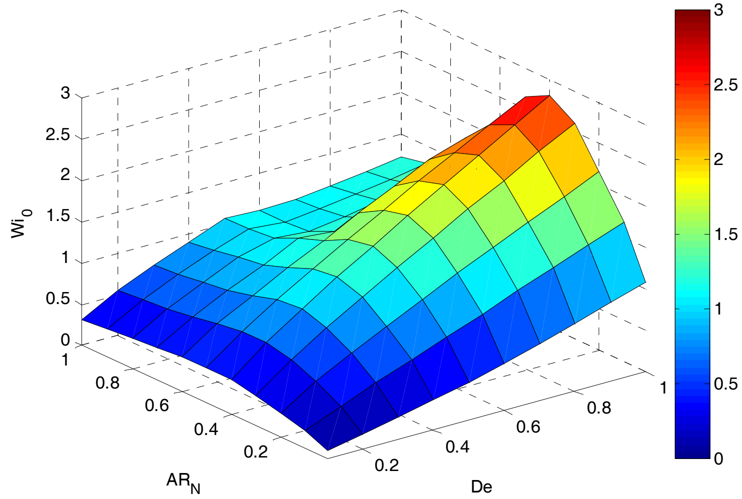
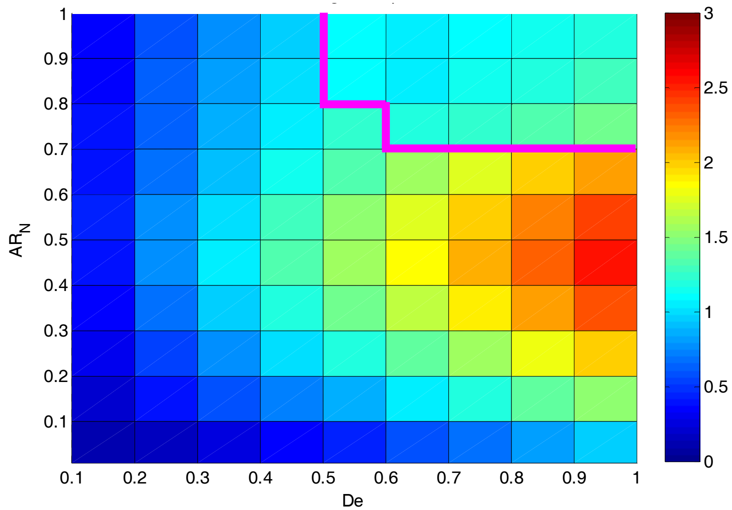
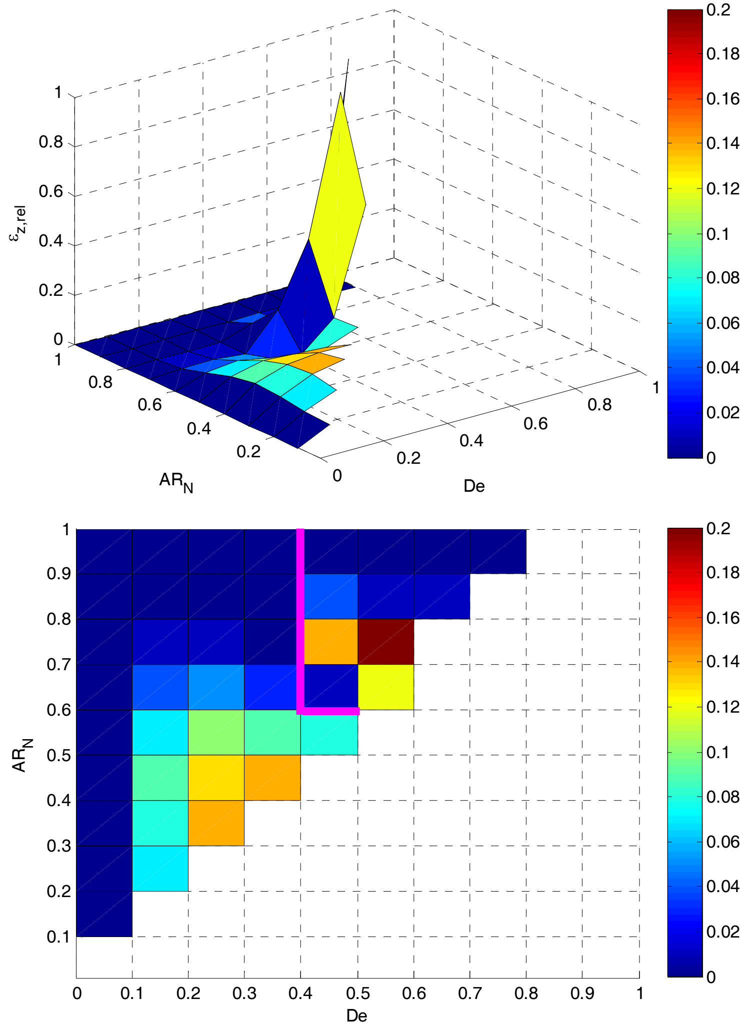




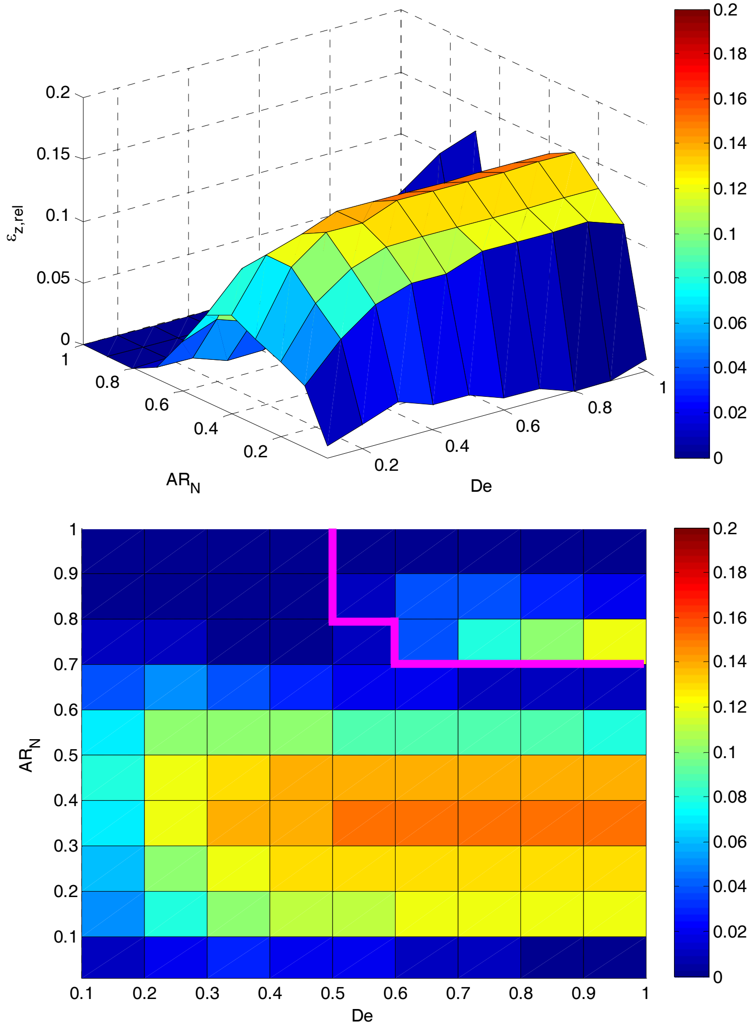
PTT: Shear-thinning; effective λ, and thus Wi, is lower than imposed λ.

Stability diagrams – Relative modulus of strain-rate along Z

UCM model

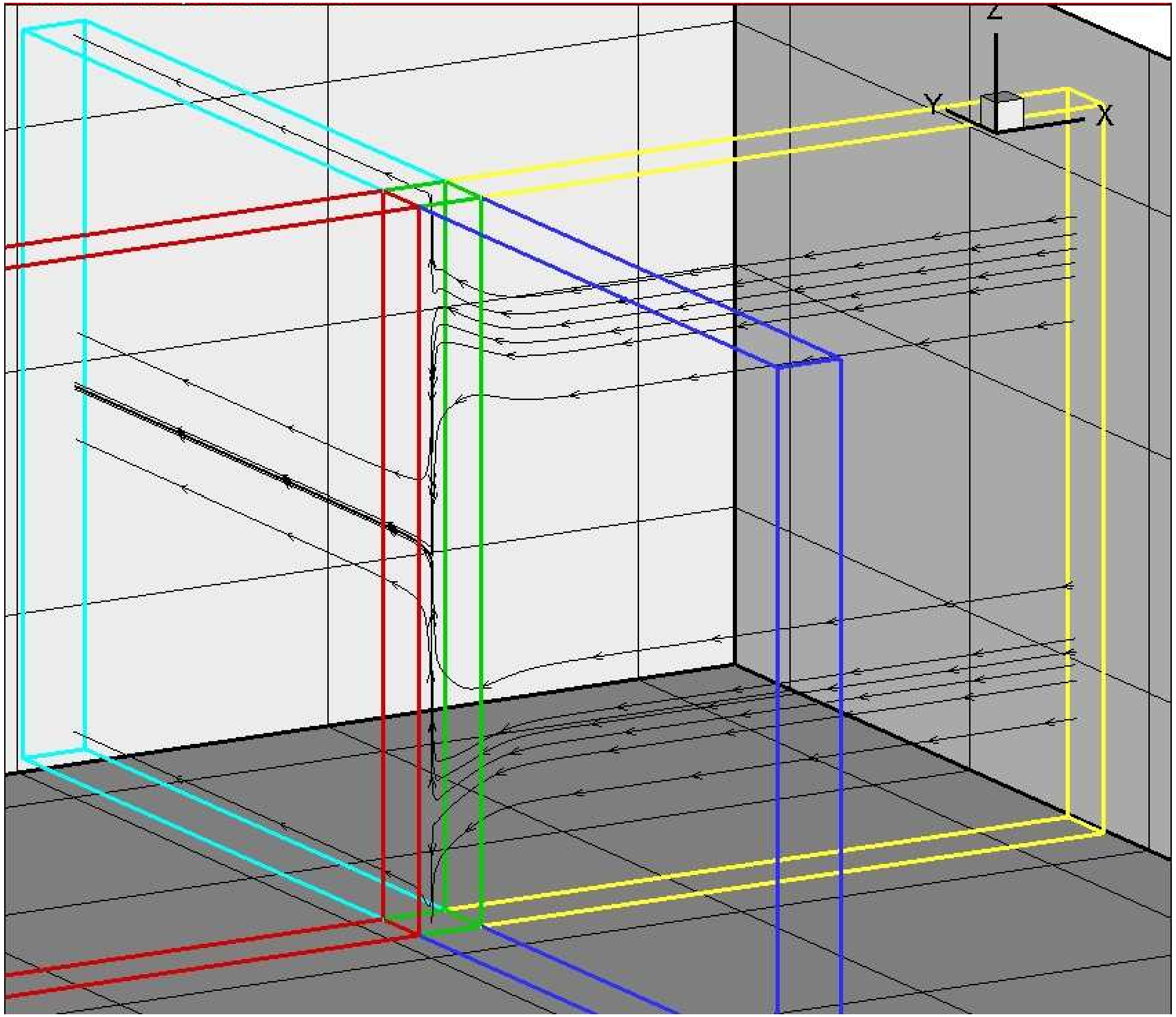


sPTT model, β=1/9, ε=0.02



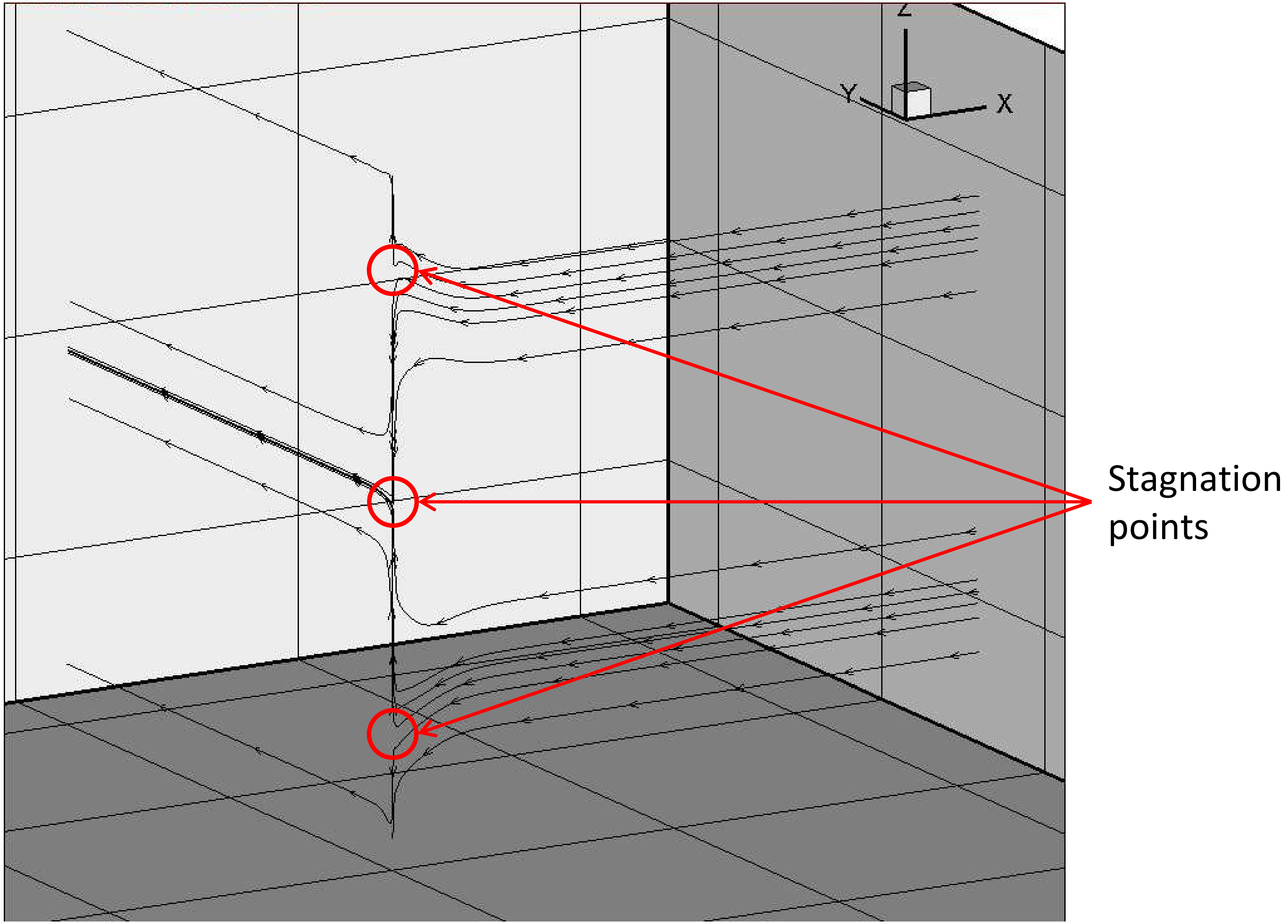
Why is the vertical strain-rate component non-negligible? Where is matter flowing from/into?

e.g. AR=1.5 (or AR_N=0.6) at De=0.6, UCM model, Asymmetric
(exaggerated Z axis)



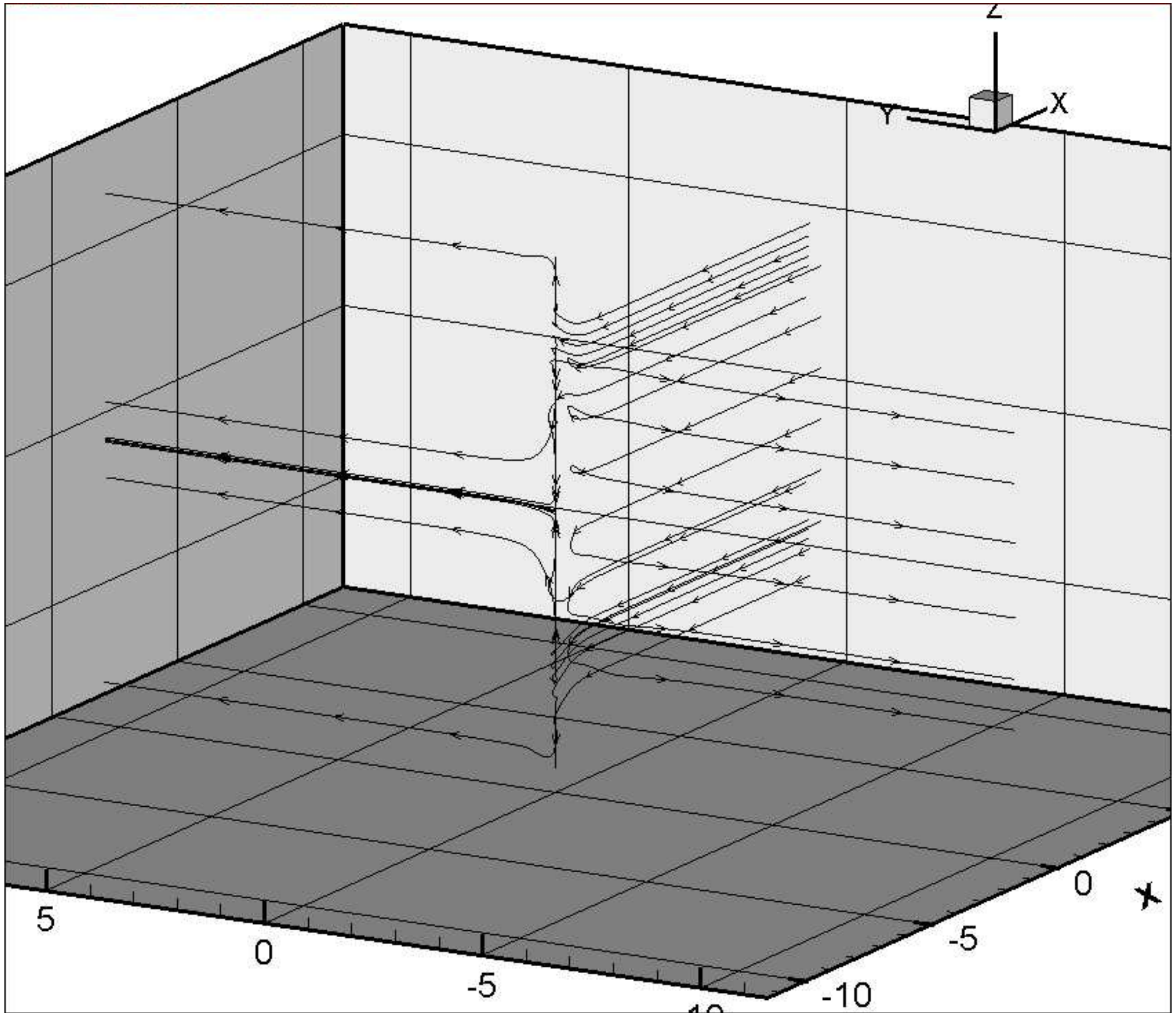
e.g. AR=1.5 (or AR_N=0.6) at De=0.6, UCM model, Asymmetric

(exaggerated Z axis)



e.g. AR=1.5 (or AR_N=0.6) at De=0.6, UCM model, Asymmetric

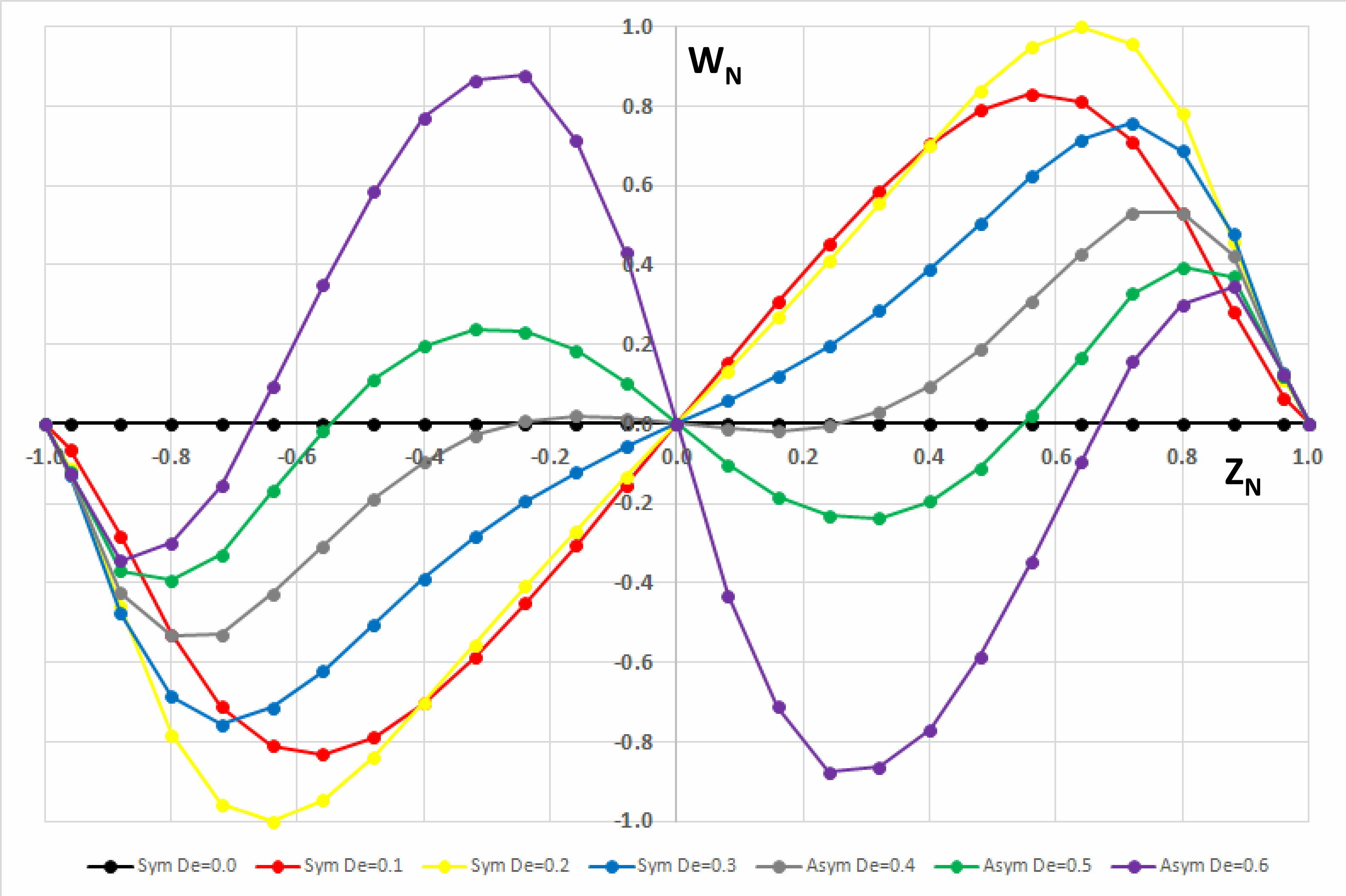
(exaggerated Z axis)



The central stagnation point is "fed" by the peripheral stagnation points.
The actual streamlines heading in its direction avoid it.

e.g. AR=1.5 (or AR_N=0.6) for all De, UCM model

Normalized velocity component w along central vertical axis z



Peripheral stagnation points form and evolve with bifurcation.

Conclusions

- 3D effects are present in cross-slot type systems and are of major importance for the understanding of elastic instabilities.
- Multiple free stagnation points form and interact with each other when the system bifurcates into a steady asymmetric configuration.
- Experimental investigations into the 3D nature of the cross-slot are needed, and should be possible at AR=0.5-1.5.

Acknowledgements

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Thank you for your attention!