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Linear stability analysis of convection in a coupled chemotaxis-fluid model

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CASTS-LJLL Workshop on Applied Mathematics

and Mathematical Sciences

May 26-29, 2014

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Outline

- Introduction
- Numerical methods
  - Nonlinear simulation
  - Linear Stability analysis
- Results
- Summary and future work

1. Introduction

Chemotaxis (from *chemo-* + *taxis*) is movement of an organism in response to a chemical stimulus.

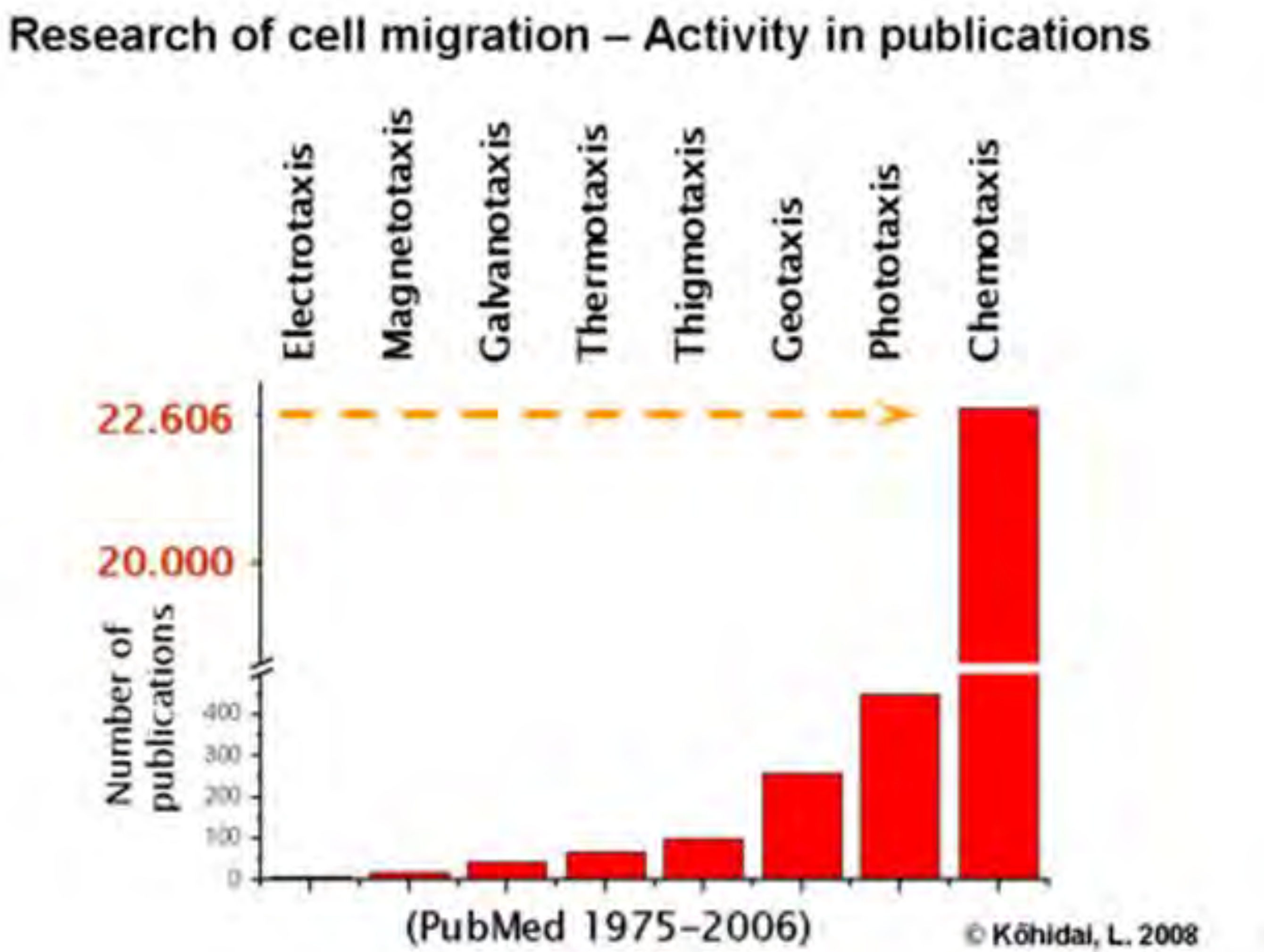
Somatic cells, bacteria, and other single cell or multicellular organisms

Importance

- For bacteria to find food (for example, glucose) by swimming toward the highest concentration of food molecules, or to flee from poisons (for example, phenol).
- In multicellular organisms, chemotaxis is critical to early development (e.g., movement of sperm towards the egg during fertilization) and subsequent phases of development (e.g., migration of neurons or lymphocytes) as well as in normal function.
- It has been recognized that mechanisms that allow chemotaxis in animals can be subverted during cancer metastasis.
- Transfer external signals to chemical signals in acupuncture.

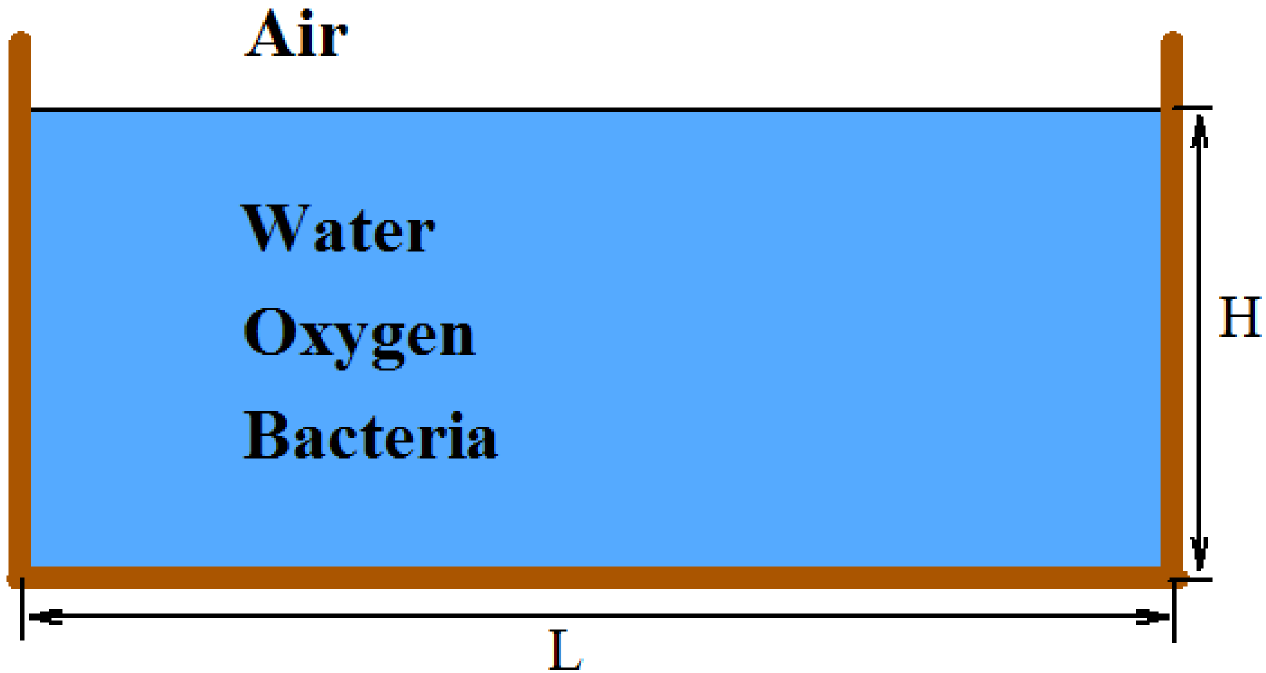
***Positive* chemotaxis** occurs if the movement is toward a higher concentration of the chemical.
***Negative* chemotaxis** occurs if the movement is in the opposite direction.

1. Introduction



Picture from wikipedia

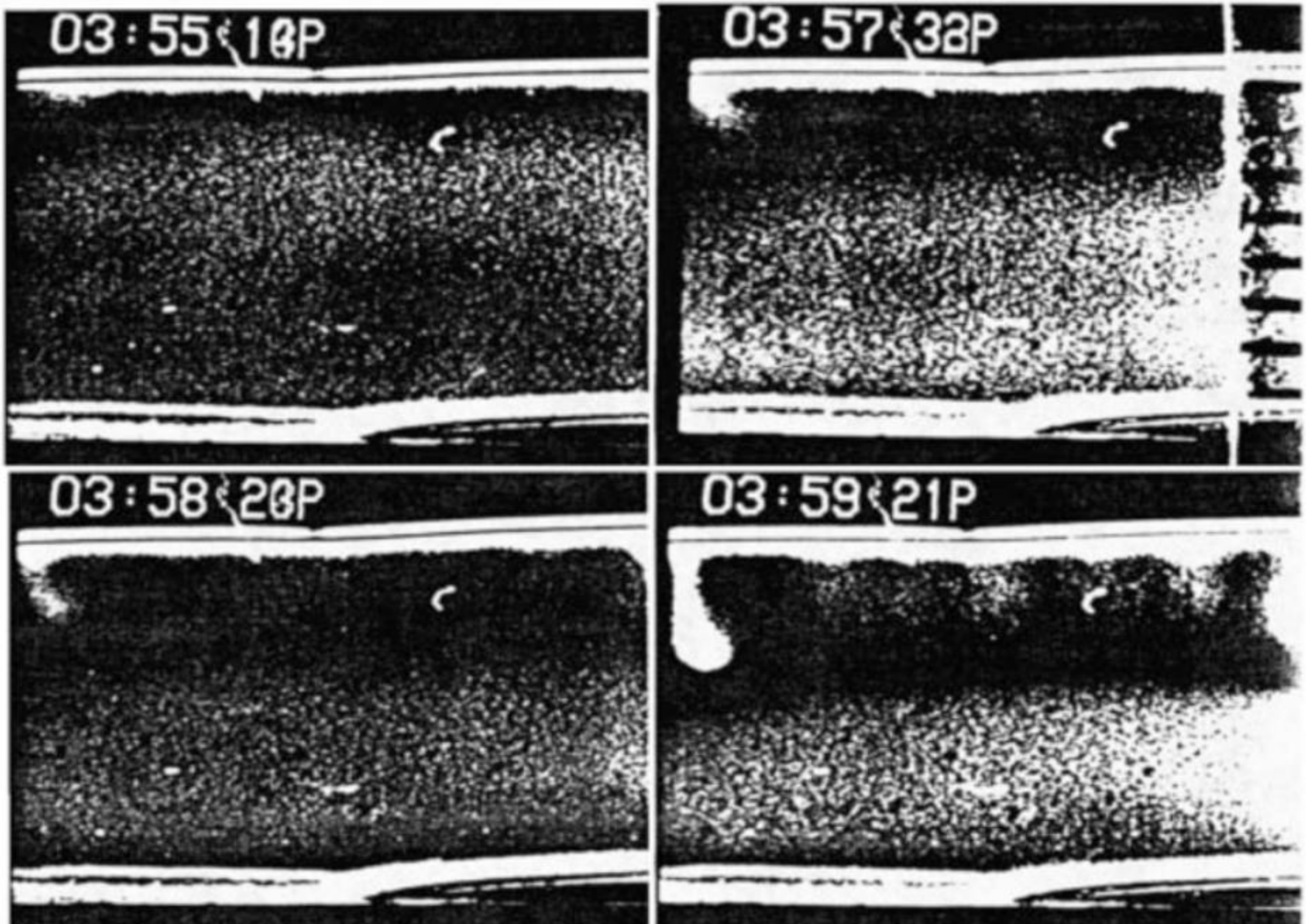
1. Introduction: bioconvection model

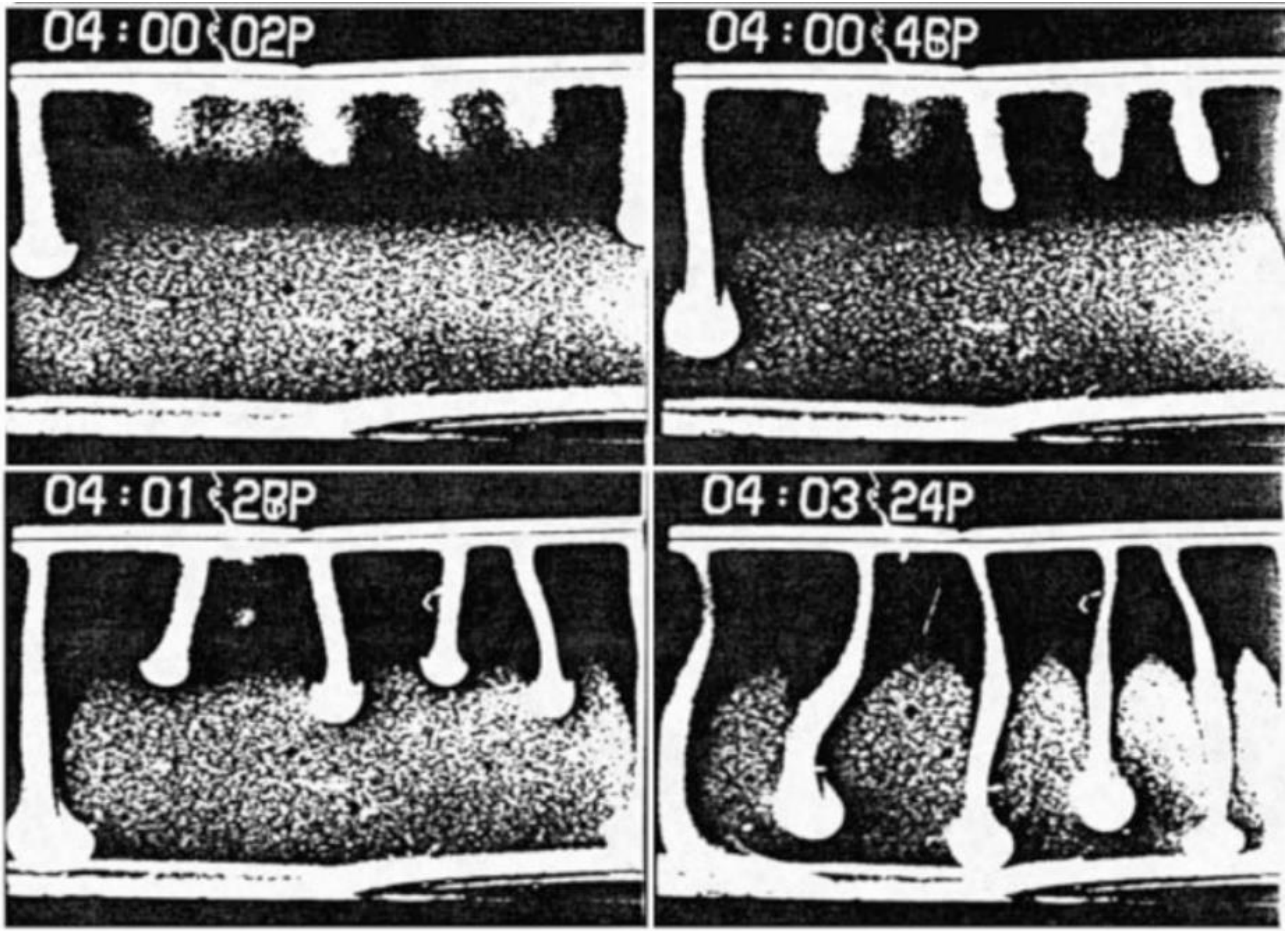


a) Bacteria cells are denser than water (about 10% denser)
b) Bacteria swim upwards on average so that the density of an initially uniform gradient becomes greater at the top than the bottom

Pattern formation in concentrated suspension of swimming bacteria (Kessler 1989)

Bacillus subtilis

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1. Introduction: bioconvection model

A. J. Hillesdon , T. J. Pedley and J. O. Kessler 1995

Neglecting

- ✓ Sedimentation and Brownian diffusion
- ✓ The biological growth and decay of the bacterial population
- ✓ The influence of rotation or straining in the ambient flow on the orientation and hence swimming direction of a cell
- ✓ The interaction between cells

$$\frac{\partial c}{\partial t}+\nabla\bullet(\boldsymbol{u}c-D_c\nabla c)=-\kappa r(c)n,$$

$$\frac{\partial n}{\partial t}+\nabla\bullet[\boldsymbol{u}n-D_n\nabla n+\chi r(c)n\nabla c]=0,$$

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\bullet\nabla\boldsymbol{u}\right)=-\nabla p+\eta\nabla^2\boldsymbol{u}-nV_b g(\rho_b-\rho)\boldsymbol{j},$$

$$\nabla\bullet\boldsymbol{u}=0.$$

κ, *oxygen consumption rate*

χ, *chemotactic sensitivity*

V_b, *volume of bacterium*

$$r(c)=\begin{cases}0, & c<c^*\\ 1, & c>c^*\end{cases}$$

Characteristic variables

Rescaling variables as follows :

$$\mathrm{x}^d = \frac{\mathrm{x}}{\mathrm{H}},\ \mathrm{t}^d = \frac{D_n}{\mathrm{H}}\mathrm{t},\ c^d = \frac{c}{c_{air}},\ n^d = \frac{n}{n_r},\ p^d = \frac{\mathrm{H}^2}{\nu\rho D_n}p,\ u^d = \frac{\mathrm{H}}{D_n}u$$

H is a characteristic length

D_n is cell diffusivity

c_{air} is oxygen concentration of the air above the fluid

n_r is characteristic cell density

ν is kinetic viscosity of fluid

ρ is density of fluid

Dimensionless governing equations

$$\frac{\partial c}{\partial t} + \nabla \bullet (\boldsymbol{u}c) = \mathrm{Le}_\tau \nabla^2 c - \mathrm{P}_\tau n,$$

$$\frac{\partial n}{\partial t} + \nabla \bullet (\boldsymbol{u}n) + \mathrm{S}_\tau \nabla \bullet (n \nabla c) = \nabla^2 n,$$

Chemotaxis

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \bullet \nabla \boldsymbol{u} = -\nabla p + \mathrm{Pr}_\tau \nabla^2 \boldsymbol{u} - \mathrm{Pr}_\tau \mathrm{Ra}_\tau n \boldsymbol{j},$$

$$\nabla \bullet \boldsymbol{u} = 0.$$

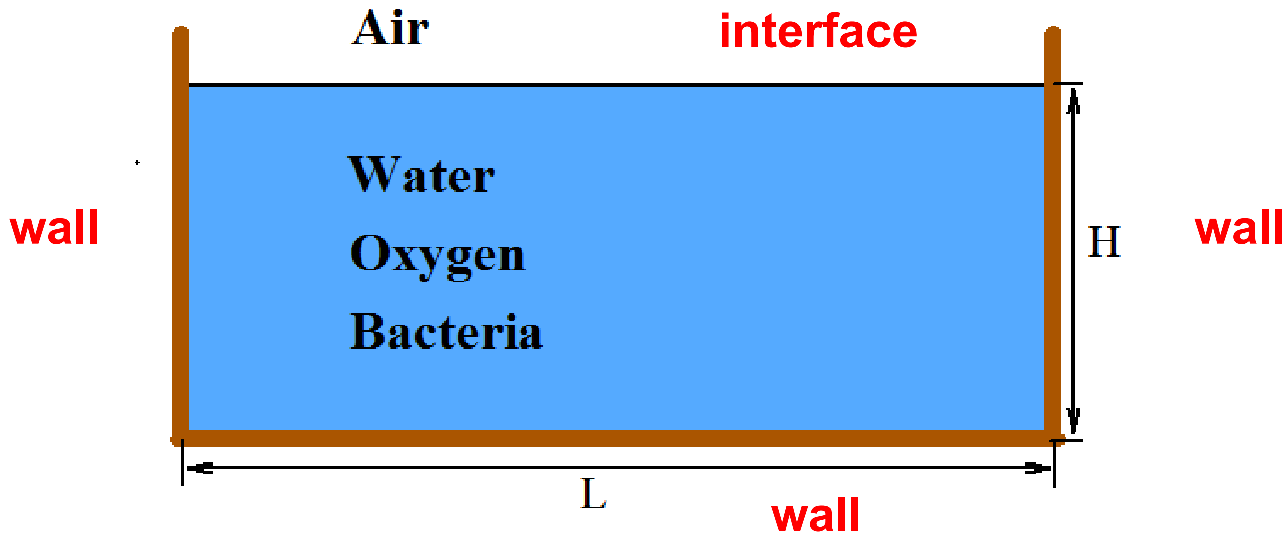
Fluid

$$\mathrm{Pr}_\tau = \frac{\nu}{D_n}, \quad \mathrm{Ra}_\tau = \frac{V_b n_\mathrm{r} g(\rho_n - \rho)\mathrm{H}^3}{\mu D_n}, \quad \mathrm{Le}_\tau = \frac{D_c}{D_n}, \quad \mathrm{S}_\tau = \frac{\chi c_{air}}{D_n}, \quad \mathrm{P}_\tau = \frac{\kappa n_\mathrm{r} \mathrm{H}^2}{c_{air} D_\mathrm{c}}$$

Taxis Prandtl number, taxis Rayleigh number, taxis Lewis number, chemotaxis sensitivity number and chemotaxis production number.

Γ=L/H, aspect ratio

Dimensionless boundary conditions



Boundary conditions:

$$S_\tau c_y n - n_y = 0,\ c = 1,\ u_y = 0,\ v = 0,\ \ at\ \ y = 1,$$ **top**

$$n_y = c_y = 0,\ \ u = 0,\ v = 0,\ \ at\ \ y = 0,$$ **bottom**

(1) *free slip side walls*

$$n_x = c_x = 0,\ \ u = 0,\ v_x = 0,\ \ at\ \ x = 0\ and\ \ x = d,$$ **side walls**

(2) *no slip side walls*

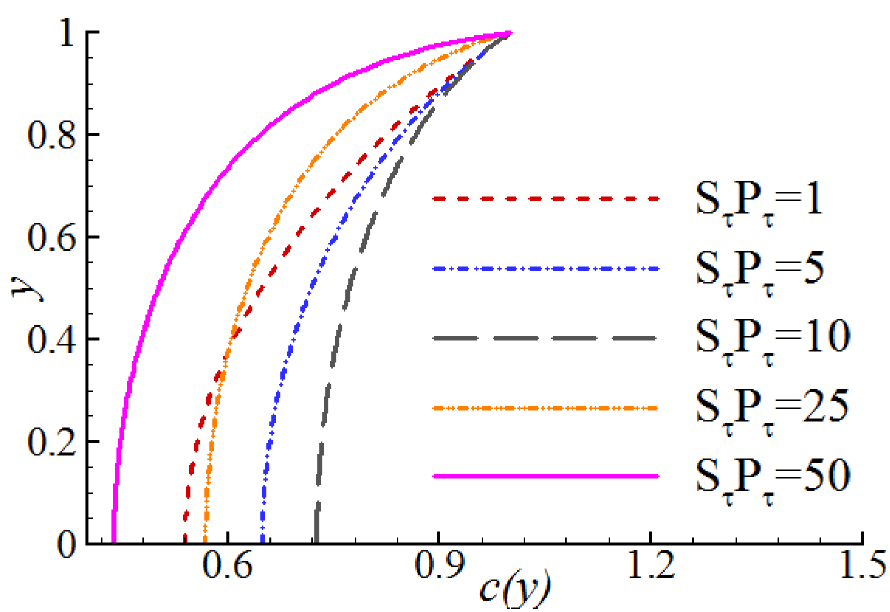
$$n_x = c_x = 0,\ \ u = 0,\ v = 0,\ \ at\ \ x = 0\ and\ \ x = d$$ **side walls**

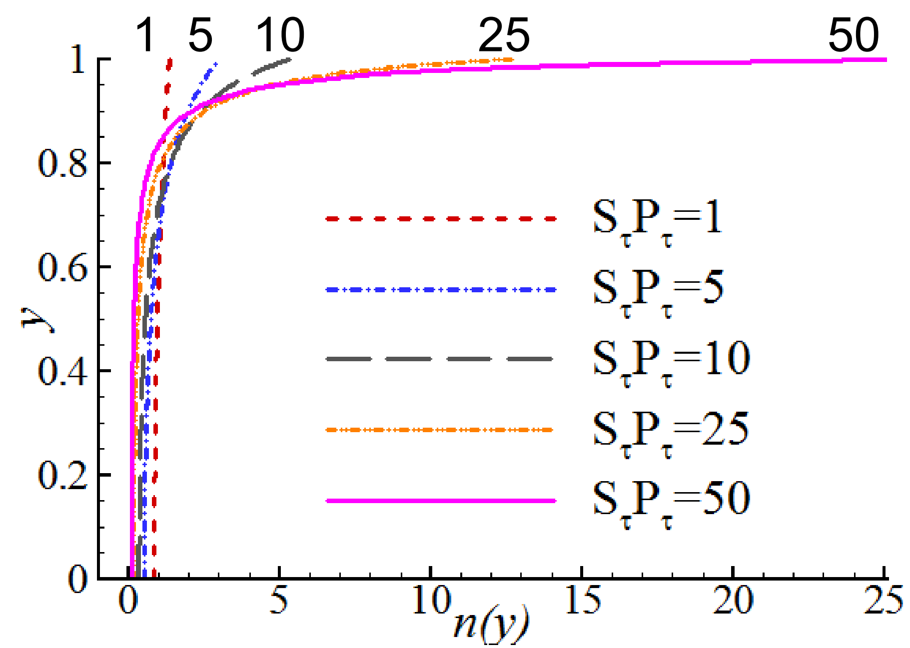
Exact solution for shallow convection: Hillesdon et al. 1995

$$c(y) = 1 - \frac{2}{S_\tau} \ln\left(\frac{\cos(\frac{S_\tau}{2} A_1 y)}{\cos(\frac{S_\tau}{2} A_1 y)} \right), \quad n(y) = \frac{A_1^2}{P_\tau} \frac{S_\tau}{2} \frac{1}{\cos^2(\frac{S_\tau}{2} A_1 y)}.$$

A_1 is a constant determined by total cell number.

Primary goal : evaluate the finite length effect (Γ) and chemotaxis effect ($S_\tau P_\tau$) on the onset of convection





2. Numerical methods

- ◆ Nonlinear simulation method
- ◆ Linear stability analysis method

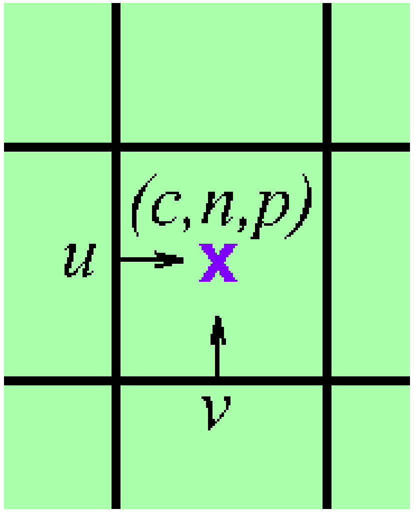
2.1 Nonlinear simulation

$$\frac{\partial n}{\partial t}+\boxed{[(u+S_\tau c_x)n]_x+[(v+S_\tau c_y)n]_y}=\boxed{\nabla^2 n},$$

$$\frac{\partial c}{\partial t}+\boxed{(uc)_x+(vc)_y}=\boxed{\mathrm{Le}_\tau \nabla^2 c}-\mathrm{P}_\tau n,$$

Second order central upwind

Second order central



$$\frac{\partial u}{\partial t}+\boxed{(u^2)_x+(uv)_y}=\boxed{\mathrm{Pr}_\tau \nabla^2 u}-p_x,$$

$$\frac{\partial v}{\partial t}+\boxed{(uv)_x+(v^2)_y}=\boxed{\mathrm{Pr}_\tau \nabla^2 v}-\mathrm{Pr}_\tau \mathrm{Ra}_\tau n-p_y.$$

Nonlinear simulation: Central upwind method

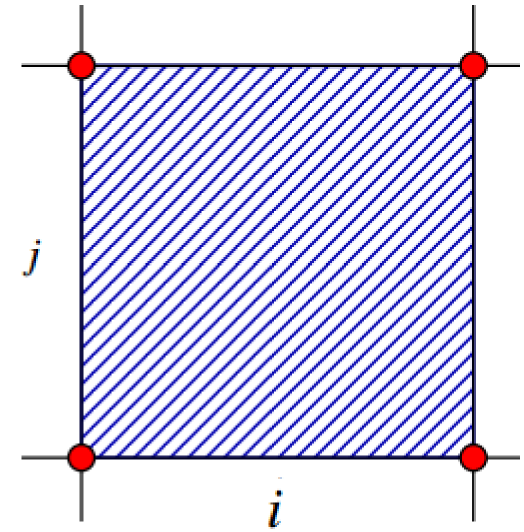
$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\frac{H^x_{i+(1/2),j} - H^x_{i-(1/2),j}}{\Delta x} - \frac{H^y_{i,j+(1/2)} - H^y_{i,j-(1/2)}}{\Delta y}$$

$$H^x_{i\pm(1/2),j} = (u + S_\tau c_x)n\,|_{(x_{i\pm(1/2)},\,y_j)}$$

$$H^y_{i,j\pm(1/2)} = (v + S_\tau c_y)n\,|_{(x_i,\,y_{j\pm(1/2)})}$$

$$H^x_{i+(1/2),j} = \begin{cases} a_{i+(1/2),j}\, n^e_{i,j} & \text{if } a_{i+(1/2),j} > 0, \\ a_{i+(1/2),j}\, n^w_{i+1,j} & \text{if } a_{i+(1/2),j} < 0, \end{cases}$$

$$H^y_{i,j+(1/2)} = \begin{cases} b_{i+(1/2),j}\, n^n_{i,j} & \text{if } a_{i+(1/2),j} > 0, \\ b_{i+(1/2),j}\, n^s_{i,j+1} & \text{if } a_{i+(1/2),j} < 0, \end{cases}$$



$$n^e_{i,j} = \bar{n}_{i,j} + \frac{\Delta x}{2}(n_x)_{i,j}, \quad n^w_{i,j} = \bar{n}_{i,j} - \frac{\Delta x}{2}(n_x)_{i,j},$$

$$n^n_{i,j} = \bar{n}_{i,j} + \frac{\Delta y}{2}(n_y)_{i,j}, \quad n^s_{i,j} = \bar{n}_{i,j} - \frac{\Delta y}{2}(n_y)_{i,j},$$

TVD Minmod2 reconstruction Is applied for derivatives

$(n_x)_{i,j}$, $(n_y)_{i,j}$

Ref. A. Chertock et al. JFM (2012), 694, pp. 155-190

Nonlinear simulation: Temporal discretization

Third order TVD Runge-Kutta (SSP-RK) schemes is used

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n), \\ u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}), \\ u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}), \end{aligned}$$

2.2 Linear stability analysis

Writing $n = \bar{n} + n'$, $c = \bar{c} + c'$, $u = \bar{u} + u'$, $v = \bar{v} + v'$, $p = \bar{p} + p'$

substitute to the control equations, we get the linearized equations,

$$\frac{\partial c'}{\partial t} + (\bar{u}c' + \bar{c}u')_x + (\bar{v}c' + \bar{c}v')_y = \mathrm{Le}_\tau \nabla^2 c' - \mathrm{P}_\tau n',$$

$$\frac{\partial n'}{\partial t} + [(\bar{u} + \mathrm{S}_\tau \bar{c}_x)n' + (u' + \mathrm{S}_\tau c'_x)\bar{n}]_x + [(\bar{v} + \mathrm{S}_\tau \bar{c}_y)n' + (v' + \mathrm{S}_\tau c'_y)\bar{n}]_y = \nabla^2 n',$$

$$\frac{\partial u'}{\partial t} + (2\bar{u}u')_x + (\bar{u}v' + \bar{v}u')_y = \mathrm{Pr}_\tau \nabla^2 u' - p'_x,$$

$$\frac{\partial v'}{\partial t} + (\bar{u}v' + \bar{v}u')_x + (2\bar{v}v')_y = \mathrm{Pr}_\tau \nabla^2 v' - \mathrm{Pr}_\tau \mathrm{Ra}_\tau n' - p'_y.$$

B.C.

$$\mathrm{S}_\tau(\bar{n}c'_y + \bar{c}_y n') - n'_y = 0,\ c' = 0,\ u'_y = 0,\ v' = 0,\ \ at\ \ y = 1,$$

$$n'_y = c'_y = 0,\ \ u' = 0,\ v' = 0,\ \ at\ \ y = 0,$$

$$n'_x = c'_x = 0,\ \ u' = 0,\ v'_x = 0,\ \ at\ \ x = 0\ and\ \ x = d$$

Linear stability analysis method

The linearized system can be written as:

$$\frac{\partial \boldsymbol{q}}{\partial t} = A\boldsymbol{q} \,,$$

where, $\boldsymbol{q} = [n', c', u', v']^T$, $A = (N_u + L)$

Assuming time exponential dependence, solution for $\boldsymbol{q}$ of the form

$$\boldsymbol{q} = [\hat{n}(\mathrm{x},\mathrm{y}), \hat{c}(\mathrm{x},\mathrm{y}), \hat{u}(\mathrm{x},\mathrm{y}), \hat{v}(\mathrm{x},\mathrm{y})]^T e^{\sigma t} = \hat{\boldsymbol{q}}(\mathrm{x},\mathrm{y})e^{\sigma t}$$

Can be sought, where the variables with a hat represent the eigenfunctions, and $\sigma = \sigma_r + i\sigma_i$, with σ_r the growth rate and σ_i its angular frequency. The eigenvalue problem is

$$A\hat{\boldsymbol{q}} = \sigma\hat{\boldsymbol{q}} \,,$$

which can be solved with corresponding boundary condition after discretization.

Linear stability analysis method

Time-stepper-based approach

Discretizing the linearized equations with first order Euler implicit method,

$$\frac{\boldsymbol{q}^{n+1}-\boldsymbol{q}^{n}}{\Delta t} = N_u(\boldsymbol{q}^n) + L(\boldsymbol{q}^{n+1}),$$

$$\begin{aligned}
\boldsymbol{q}^{n+1} &= (\mathrm{I}-\Delta tL)^{-1}(\Delta tN_u + \mathrm{I})\boldsymbol{q}^n \\
&= (\mathrm{I}-\Delta tL)^{-1}(\Delta tN_u + \Delta tL + \mathrm{I}-\Delta tL)\boldsymbol{q}^n \\
&= \boldsymbol{q}^n + \Delta t(\mathrm{I}-\Delta tL)^{-1}(N_u + L)\boldsymbol{q}^n \\
&\simeq \boldsymbol{q}^n + \Delta t(N_u + L)\boldsymbol{q}^n \qquad (\Delta t << 1) \\
&\simeq e^{\Delta t(N_u+L)}\boldsymbol{q}^n \\
&= \boxed{e^{\Delta tA}\boldsymbol{q}^n}
\end{aligned}$$

Arnoldi's method is used to obtain the leading eigenvalues of $e^{\Delta tA}$, thus the eigenvalues of *A* can be obtained (Arpack).

Ref. Annual review 2011, V. Theofilis, Global Linear Instability.

Numerical test- nonlinear simulation

A comparison between analytical and numerical solution

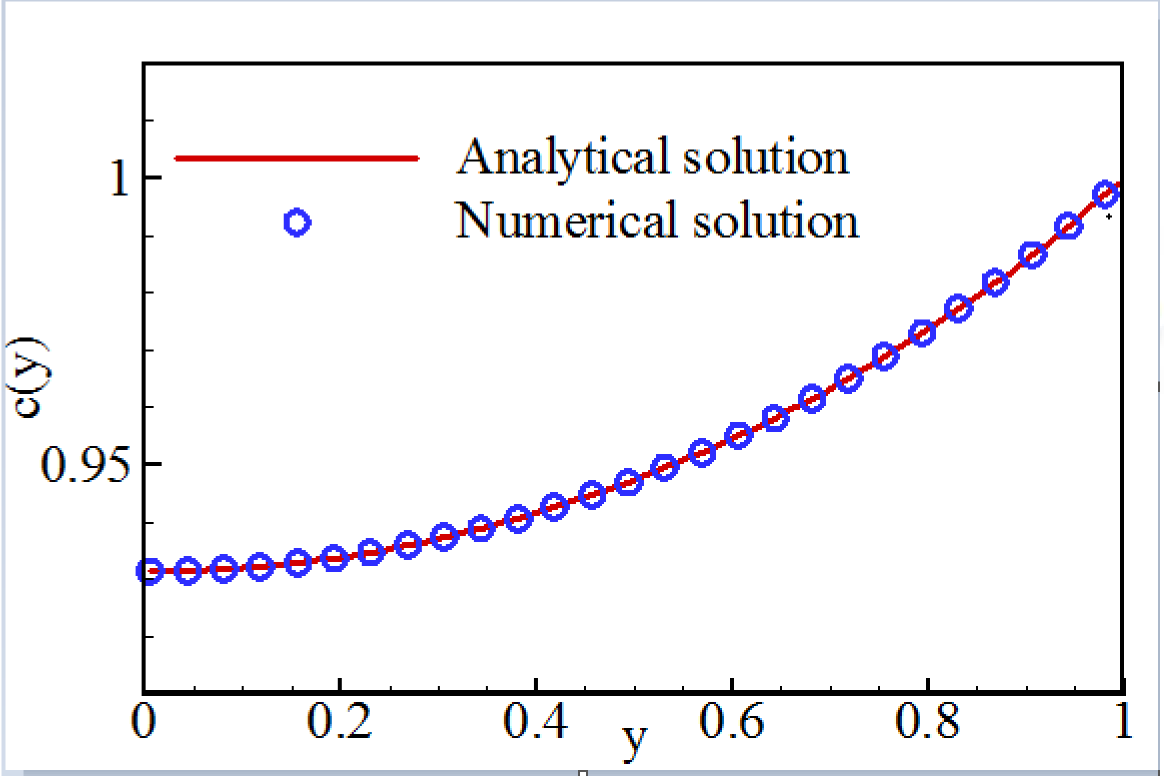
Ny=50

$S_\tau = 10$

$P_\tau = 10$

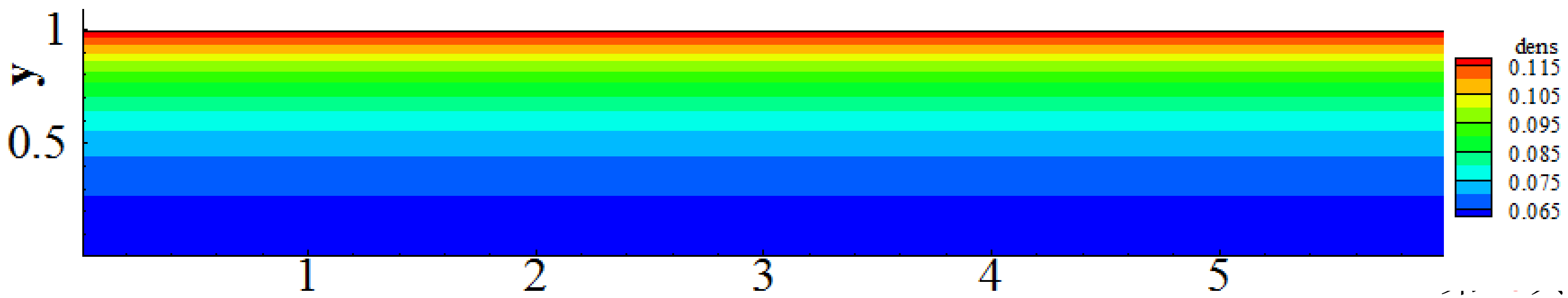
$Le_\tau = 5$

$A = \pi / 20$



$$n_0(x, y) = \frac{\pi}{40}$$

$$c_0(x, y) = 1$$



Numerical test- nonlinear simulation

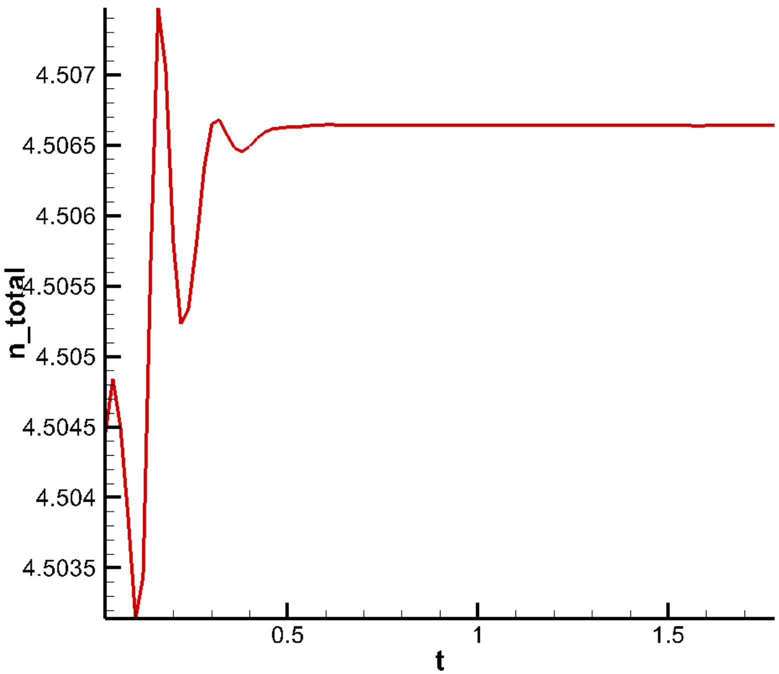
Comparison of present results with FEM results.

Initial conditions:

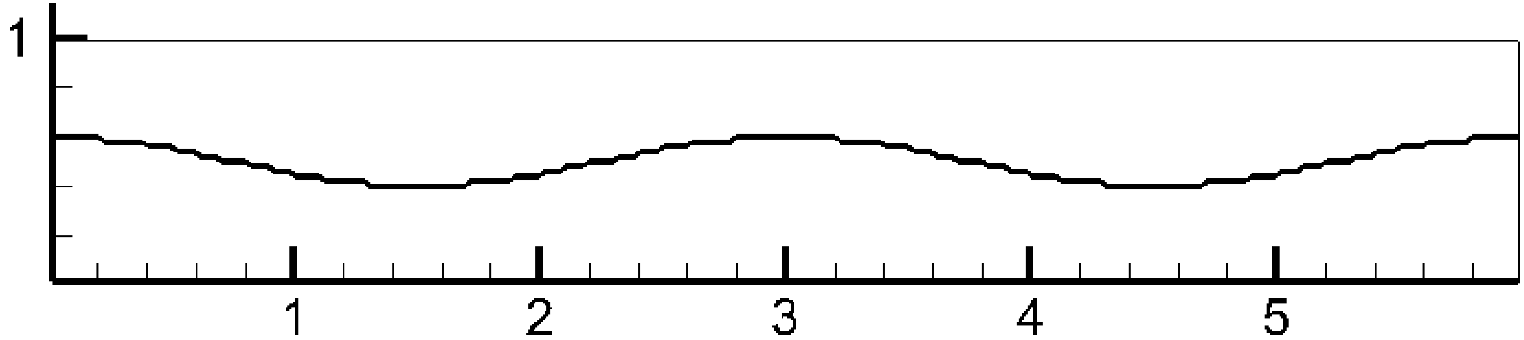
$$n_0 = \begin{cases} 1, \ y \geq 0.5+0.1\cos(\dfrac{2\pi x}{3}) \\ 0.5, \ y < 0.5+0.1\cos(\dfrac{2\pi x}{3}) \end{cases}$$

$$c_0 = 1$$

$$u_0 = 0, v_0 = 0$$



n_total increase 0.14%



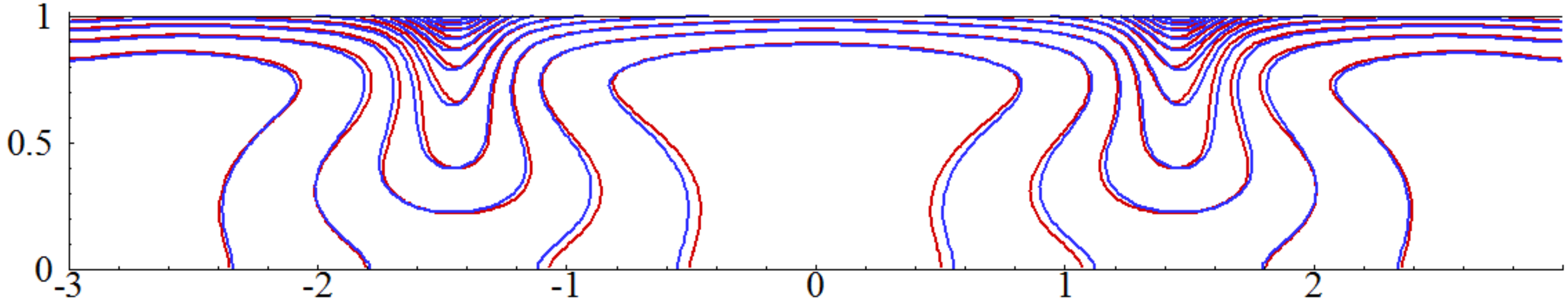
In the following, blue lines represent FEM result and red lines indicate present FVM result

- Comparison of cell distribution. (contours of *n*)

grid 40X240 50X300

The value of blue line is in (0.3854-2.8266)

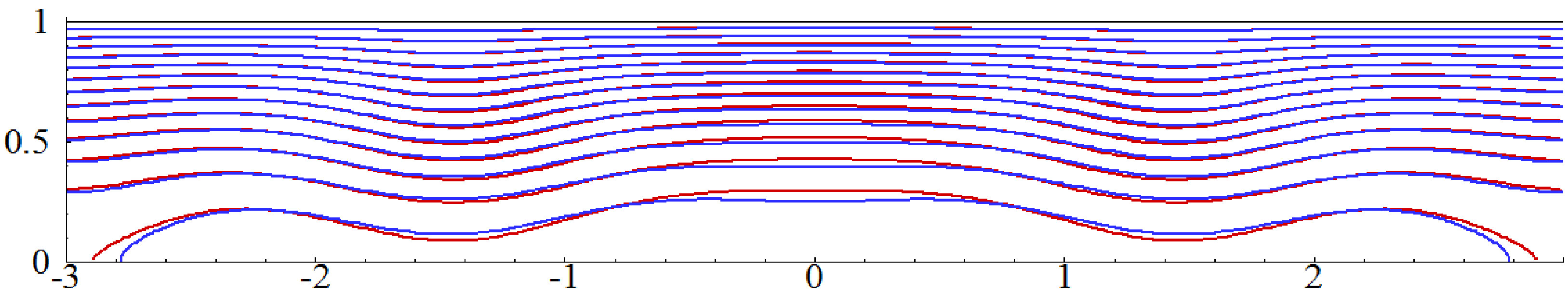
The value of red line is in (0.3873-2.6346)



- Comparison of oxygen distribution.(contours of *c*)

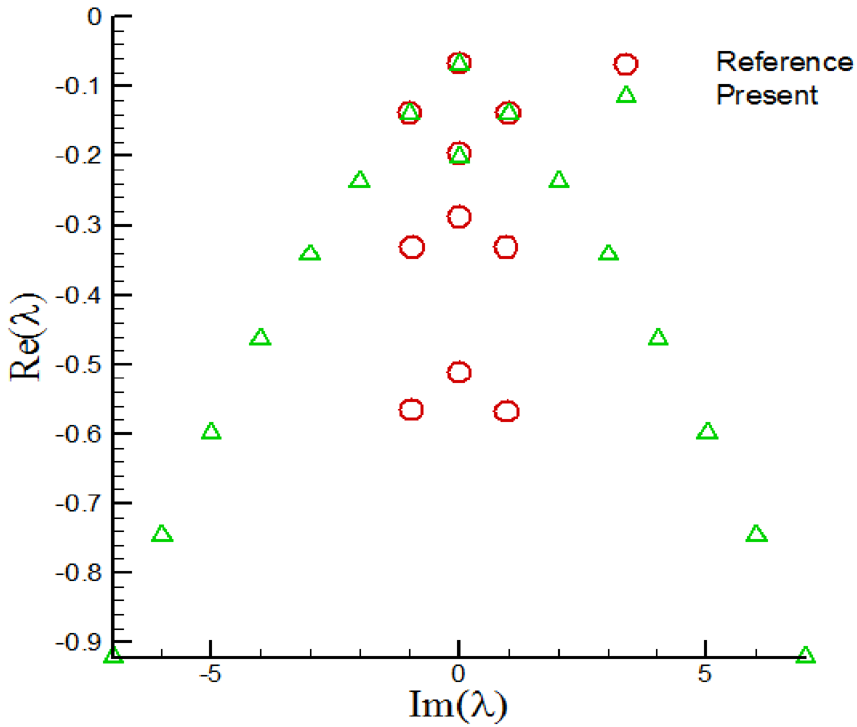
The value of blue line is in (0.7255-1)

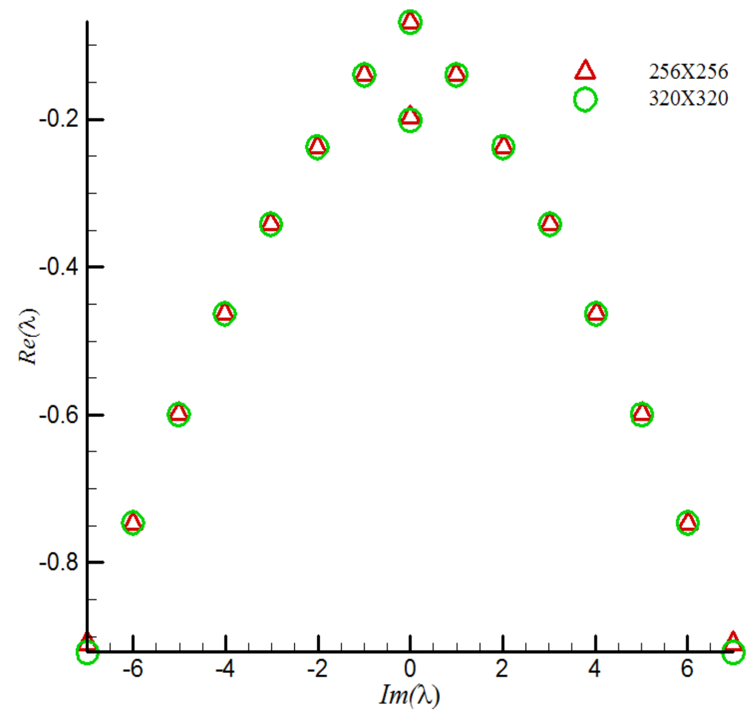
The value of red line is in (0.7225-1)



Numerical test- Linear stability analysis

Lid-driven cavity flow， Re=1000



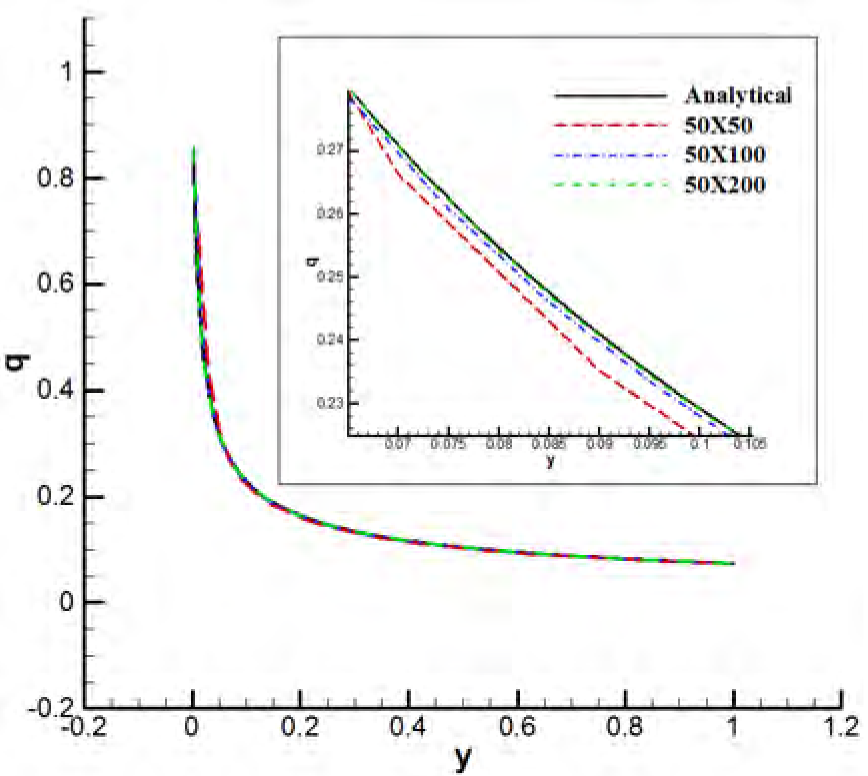


	leading eigenvalue (most unstable)
Reference	-0.0680717
Second central (256X256)	-0.0680663
Second central (320X320)	-0.0680747

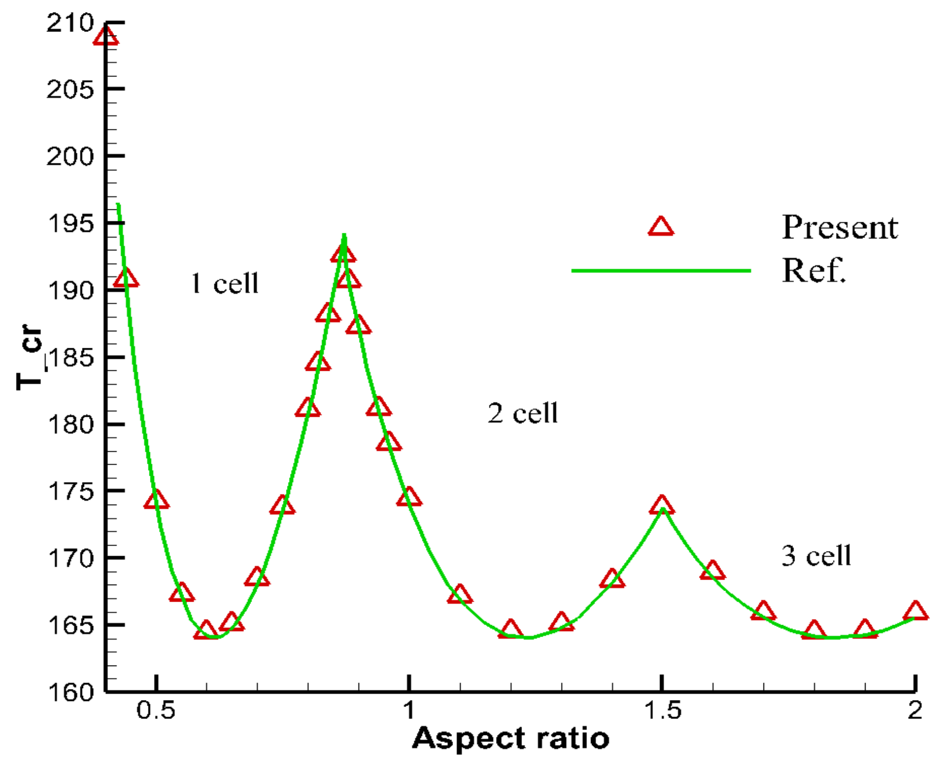
Ref. Xavier Merle et al. Computer & Fluids (2010) 39, 911-925

Numerical test- Linear stability analysis

Unipolar injection， C=10



Base flow



Stability curve

Ref. Wu Jian et al. PRE E88 053018 (2013)

Numerical test- Linear stability analysis

Bioconvection in suspension of oxytancitic baccteria

Le_τ	$S_\tau P_\tau$	Ra_{cr}(ref.)	Ra_{cr}(Pres.)	Discrepancy
1	0.05	10200	10205	0.05%
1	1	625	624	0.16%
1	10	200	200.1	0.05%
1	50	328	325	0.91%
1	100	522	522.4	0.077%
10	10	241	238	1.2%

Ref. A. J. Hillesdon and T. J. Pedley JFM (1996), 324, pp. 223.

The horizontal direction is periodic in this paper. In present computation, free slip wall boundary is used and L=6*λc*, where *λc* is critical wave length in horizontal direction.

Control parameters setting

Initial cell concentration	$N_0 \approx 10^9\ \mathrm{cm}^{-3}$
Initial oxygen concentration	$C_0 \approx 1.5 \times 10^{17}$ molecules cm^{-3}
Max. cell diffusivity	$D_{N0} \approx 1.3 \times 10^{-6}\ \mathrm{cm}^2\ \mathrm{s}^{-1}$
Max. cell swimming speed	$V_{s0} \approx 2 \times 10^{-3}\ \mathrm{cm\ s}^{-1}$
Oxygen diffusivity	$D_c \approx 2.12 \times 10^{-5}\ \mathrm{cm}^2\ \mathrm{s}^{-1}$
Chemotaxis constant	$a \approx \min\ (0.1h,\ 0.05\ \mathrm{cm})$
Max. oxygen consumption rate	$K_0 \approx 10^6$ molecules $\mathrm{cell}^{-1}\ \mathrm{s}^{-1}$
Cell density ratio	$(\rho_c - \rho_w)/\rho_w \approx 0.1$
Dynamic viscosity	$\mu \approx 10^{-2}\ \mathrm{g\ cm}^{-1}\ \mathrm{s}^{-1}$
Cell volume	$v \approx 10^{-12}\ \mathrm{cm}^3$
Density of water	$\rho_w \approx 1.0\ \mathrm{g\ cm}^{-3}$
Kinematic viscosity	$\nu \approx 10^{-2}\ \mathrm{cm}^2\ \mathrm{s}^{-1}$

TABLE 1. Estimates of typical dimensional parameters for a suspension of *Bacillus subtilis*.

A. J. Hillesdon and T. J. Pedley **JFM** 1996

Tuval et al. **Proc. Natl Acad. Sci.** 2005

$S_\tau = 10,\ Le_\tau = 5,\ Pr_\tau = 500$

The estimation of dimensionless parameters

$$\mathrm{Le}_{\tau} = \frac{D_c}{D_n}, 2\text{-}20$$

$$\mathrm{Pr}_{\tau} = \frac{\nu}{D_n}, \text{ varies with } \mathrm{Le}_{\tau}$$

$$\mathrm{Ra}_{\tau} = \frac{V_n n_\mathrm{r} g(\rho_n - \rho)\mathrm{L}^3}{\mu D_n}, \ 10^2\text{-}10^4$$

$$\mathrm{S}_{\tau} = \frac{\chi c_{air}}{D_n}, 10\text{-}100$$

$$\mathrm{P}_{\tau} = \frac{\kappa n_\mathrm{r} \mathrm{L}^2}{c_{air} D_\mathrm{c}}, 7\text{-}200$$

$$\mathrm{Le}_{\tau} = 5$$

$$\mathrm{Pr}_{\tau} = 500$$

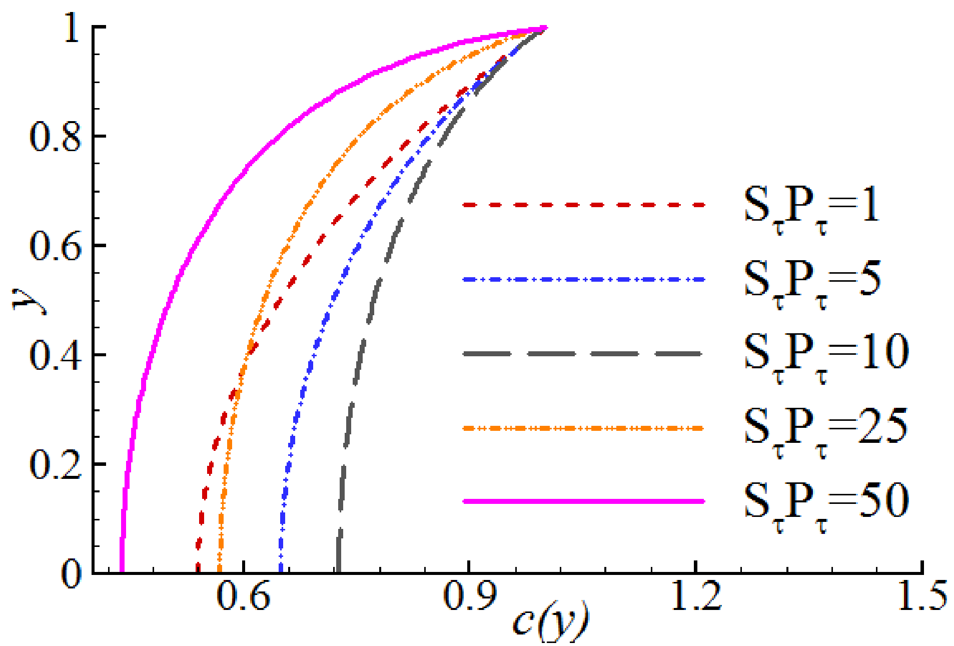
$$\mathrm{S}_{\tau}\mathrm{P}_{\tau} = 1\text{-}50$$

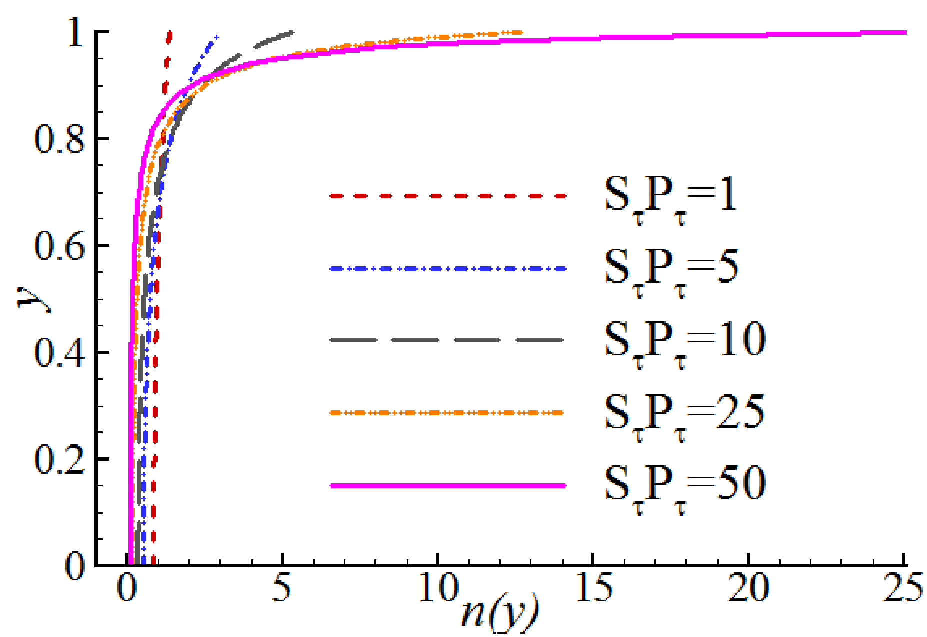
$$\Gamma = 1\text{-}8$$

3. Linear stability results

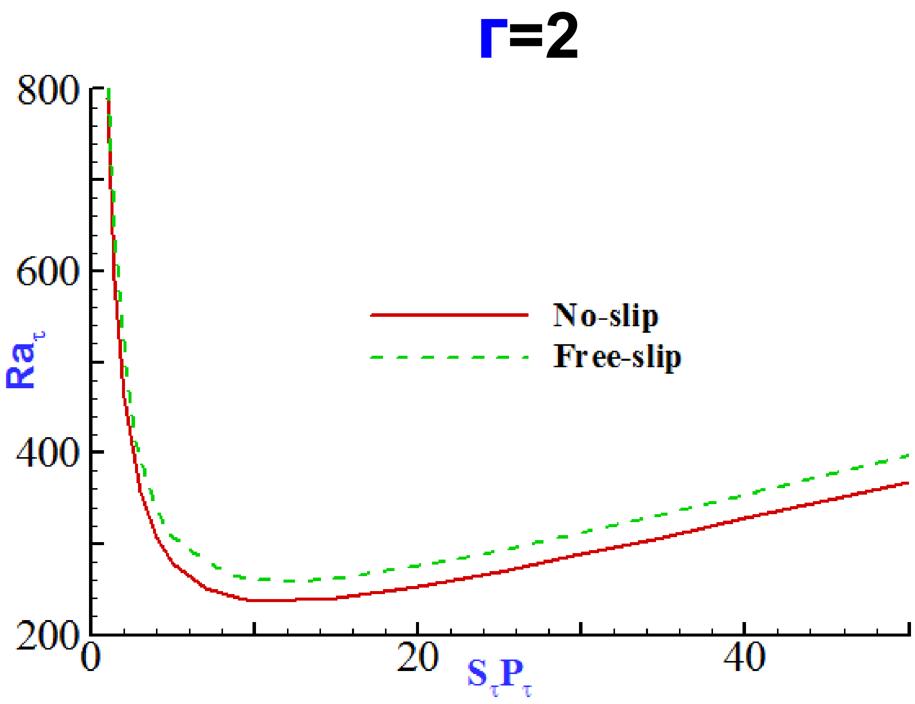
Base flow:

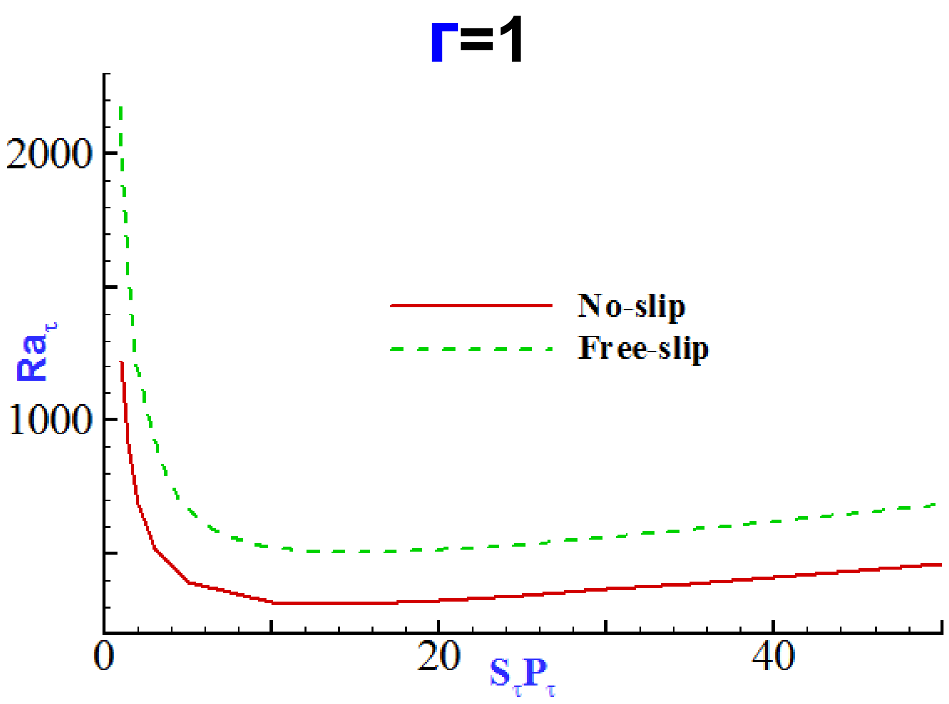
$$\bar{c}(y) = 1 - \frac{2}{S_\tau} \ln\left(\frac{\cos(\frac{S_\tau}{2} A_1 y)}{\cos(\frac{S_\tau}{2} A_1 y)} \right), \quad \bar{n}(y) = \frac{Le_\tau A_1^2}{P_\tau} \frac{S_\tau}{2} \frac{1}{\cos^2(\frac{S_\tau}{2} A_1 y)}.$$



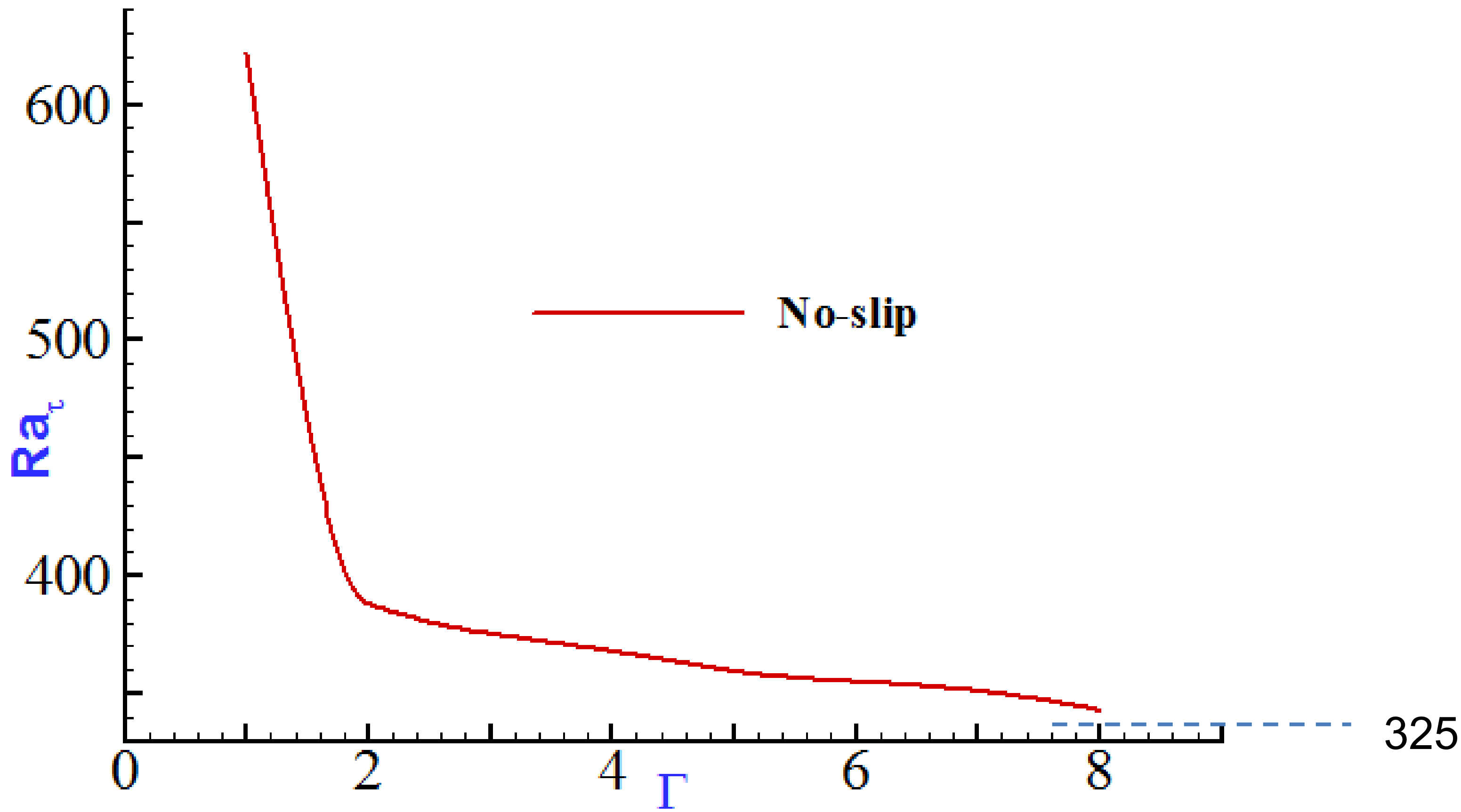


3. Linear stability results





3. Linear stability results



$S_T P_T$=50

Summary

- ✓ A matrix-free method is adapt to analysis linear instability of a bioconvection system
- ✓ Chemotaxis driven convection is much different from thermal convection
- ✓ Sidewall boundary condition has less effect on flow instability when **Γ** is large and **$S_T P_T$** is small

Future work

- ✓ Linear stability of deep convection
- ✓ Numerical simulation of nonlinear development of flow patterns

Thank you！