Project Options for SHONM2013

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Abstract

Several topics are presented to be your choice of final project. You can choose 1.1,1.2, 2, 3.1, 3.2 as your final project or something from your own research experience. You are encouraged to discuss these topics with each other but please finish the project by your own. You should fix down the topic beofre June 18, and finish it by July 9. Each one will be given 15 minutes to present your work in the last class meeting on July 10.

Please feel free to contact me (hyu@lsec.cc.ac.cn, office: Z210) if you have questions on the final project.

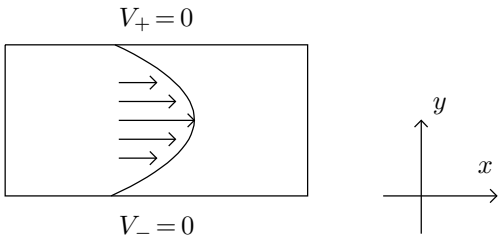
1 Navier–Stokes Solver for Special Domains

We consider the 2-dimensional Navier–Stokes equation

$$\begin{cases} \vec{u}_t + \vec{u}\cdot\nabla\vec{u} + \nabla p = \frac{1}{\mathrm{Re}}\Delta\vec{u} + \vec{f}\,, \\ \nabla\cdot\vec{u} = 0, \end{cases} \tag{1}$$

in different special domains.

1. Poiseuille flow in rectangular domain. $\vec{x} = (x, y) \in [0, L] \times [-1, 1]$.



   a. The solution satisfies the non-slip boundary condition on $y = \pm 1$, and periodic in x. i.e.

$$\vec{u}\,(x, y = \pm 1) = \begin{pmatrix} V_\pm \\ 0 \end{pmatrix}, \quad \vec{u}\,(x + L, y) = \vec{u}\,(x, y).$$

   To drive the flow, we set

$$\vec{f} = \begin{pmatrix} C \\ 0 \end{pmatrix}, \quad C = \frac{2}{\mathrm{Re}}.$$

   b. Non-slip boundary condition on $y = \pm 1$, and Dirichlet condition on $x = 0$ and Neumann condition on $x = L$. i.e.

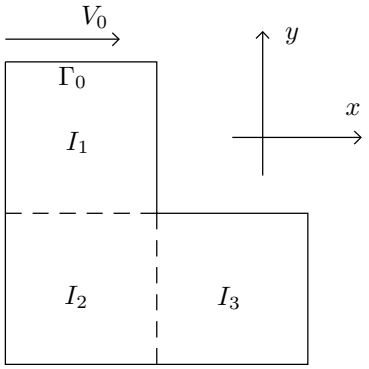
$$\vec{u}\,(x, y = \pm 1) = \begin{pmatrix} V_\pm \\ 0 \end{pmatrix}, \quad \vec{u}\,(0, y, t) = \begin{pmatrix} U(y,t) \\ V(y,t) \end{pmatrix}, \quad \frac{\partial}{\partial x}\vec{u}\,(x, y, t)|_{x=L} = 0.$$

   In this boundary condition, we set $\vec{f} = \vec{0}$.

For these two kind of boundary conditions design propriate spectral methods. Some temporal discretization schemes for Navier-Stokes equation is discussed in Section 9.4 of ShenTangWang's 2011 book.

For the periodic case, when Reynold number Re is small, the solution converge to $u(x, y) = U(y) = 1 - y^2$. But for a larger Re number, $\mathrm{Re} > R_G$, $U(y)$ is not the unique solution, when Re get large enough, see $\mathrm{Re} > R_\star$, $U(y)$ is not stable anymore. Try use the spectral solver to fix R_G and $R\star$.

2. L-shaped cavity flow.



$$\Omega = I_1 \cup I_2 \cup I_3$$

$$I_1 = [-1,0] \times [0,1]$$
$$I_2 = [-1,0] \times [-1,0]$$
$$I_3 = [0,1] \times [-1,0]$$

$$\Gamma_0 = [-1,0] \times \{1\}$$
$$\bar{\Gamma} = \partial\Omega \backslash \Gamma_0$$

with boundary condition

$$\vec{u}\Big|_{\Gamma_0} = \begin{pmatrix} c(t)V_0 \\ 0 \end{pmatrix}, \quad \vec{u}\Big|_{\bar{\Gamma}} = \vec{0},$$

where

$$c(t) = \begin{cases} \frac{t}{T}, & 0 \leqslant t < T, \\ 1, & t \geqslant T. \end{cases}$$

Implement a spectral element solver using three square elements to solver the system. Compare the solution for $V_0 > 0$ and $V_0 < 0$.

2 Linear Schrödinger Equation for Electronic Structure

The basic equation in the quantum mechnics is the Schrödinger equation. Here we consider the Schrödinger equation for the electronic distribution in an atom.

$$H\psi := -\frac{1}{2}\sum_{i=1}^{n} \Delta_i \psi + V(\vec{x}_1, ..., \vec{x}_n)\psi = E\psi, \tag{2}$$

where $\psi(\vec{x}_1, ..., \vec{x}_n) \in H^1(\mathbb{R}^{dn})$ is the so-called wavefunction, $\vec{x}_i \in \mathbb{R}^d$ for each i. d is the number of dimensions. n is the number of electrons. For simplicity, we only study the case $d = 1$ or 3 and $n = 1$ or 2. $V(\vec{x}_1, ..., \vec{x}_n)$ is the potential. Equation (2) is an eigenvalue problem. Eigenvalue E is the energy. $V(\vec{x}_1, ..., \vec{x}_n)$ is given by

$$V = \begin{cases} Z\sum_{i=1}^{n} |x_i| - \sum_{i<j} |x_i - x_j|, & d = 1, \\ -Z\sum_{i=1}^{n} \frac{1}{|\vec{x}_i|} + \sum_{i<j} \frac{1}{\left|\vec{x}_i - \vec{x}_j\right|}, & d = 3. \end{cases}$$

Here $|\cdot|$ denotes the Euclidean distance in $\mathbb{R}^d$, Z is the number of electronic charge of nucleus.

1. 1-D case.

   a. One electron (n=1).

   $$-\frac{1}{2}\psi'' + Z|x|\psi = E\psi, \qquad \psi(x) \in H^1(\mathbb{R}).$$

   b. Two electrons (n=2)

   $$-\frac{1}{2}\Delta\psi + Z(|x_1| + |x_2|)\psi - |x_1 - x_2|\psi = E\psi, \quad \psi(x_1, x_2) \in H^1(\mathbb{R} \times \mathbb{R})$$

2. 3-D case.

   a. One electron ($n = 1$)

   $$-\frac{1}{2}\Delta\psi - \frac{Z}{|\vec{x}|}\psi = E\psi, \quad \psi(\vec{x}) \in H^1(\mathbb{R}^3)$$

b. Two electrons ($n=2$)

$$-\frac{1}{2}(\Delta_1+\Delta_2)\psi-\frac{Z}{|\vec{x}_1|}\psi-\frac{Z}{|\vec{x}_2|}\psi+\frac{1}{|\vec{x}_1-\vec{x}_2|}\psi=E\psi,\quad \psi(\vec{x}_1,\vec{x}_2)\in H^1(\mathbb{R}^3\times\mathbb{R}^3)$$

Design spectral methods (Laguerre, Legendre on truncated domain) to calculate the first several eigenvalue to high accuracy for $d=1,n=1,2$ case. For 3-D case, you can design efficient algorithm if you have some idea, no need to finish the implementation and get the computing results.

3 Fokker-Planck Equation for Polymer Dynamics

3.1 Rodlike polymer (Liquid Crystal Polymer)

Suppose some rod-like polymer solution or melt orientationare stored in a container. Let $f(\vec{x},\vec{m},t)$ be the probality of finding a polymer at position $\vec{x}$ with orientation $\vec{m}$ at time t. $\vec{x}\in\mathbb{R}^d$, d is the number of dimension. $\vec{m}$ is the orientation vector in d-dimension, i.e. $\vec{m}\in\mathbb{R}^d$ and $|\vec{m}|=1$. Assume that the two ends of the molecules are indistinguishable, i.e. $f(\vec{x},\vec{m},t)=f(\vec{x},-\vec{m},t)$.

For simplicity, we only study spatial homogeneous system, i.e. $f(\vec{x},\vec{m},t)=f(\vec{m},t)$. The dynamics of system is described by the so-called Doi-Smoluchowski [M. Doi and S. F. Edwards, The Theory of Polymer Dynamics, Oxford 1986]:

$$\frac{\partial f}{\partial t}=\frac{1}{\mathrm{De}}\mathcal{R}\cdot(\mathcal{R}f+f\mathcal{R}U)-\mathcal{R}\cdot(\vec{m}\times(\kappa\cdot\vec{m})f),\quad \vec{m}\in\Omega:=\{\vec{m}\in\mathbb{R}^d,|\vec{m}|=1\} \tag{3}$$

where $\mathcal{R}$ is the gradient operator on sphere, $\kappa=(\nabla u)^T$ is the shear strain tensor, non-dimensional constant De is the Debroah number. U is the mean-field intermolecular potential, there are two potential that mostly accepted in the literature. One is Maier-Saupe potential, the othor one is Onsager potential:

$$U_{\mathrm{MS}}(\vec{m},t)=U_0\int_\Omega|\vec{m}\times\vec{m}'|^2f(\vec{m}',t)\,\mathrm{d}\vec{m}' \tag{4}$$

$$U_{\mathrm{OS}}(\vec{m},t)=U_0\int_\Omega|\vec{m}\times\vec{m}'|f(\vec{m}',t)\,\mathrm{d}\vec{m}' \tag{5}$$

Equation (3) is the equation for 3-dimensional case. For 2-dimensional case, $\vec{m}=(\cos\theta,\sin\theta,0)^T$, density function f depends only on θ and t. We still denote it by $f(\theta,t)$. And further assume that

$$\kappa=\begin{pmatrix}0&u_y\\0&0\end{pmatrix},$$

then equation (3) is reduced to

$$\frac{\partial f}{\partial t}=\frac{1}{\mathrm{De}}\partial_\theta(\partial_\theta f+f\,\partial_\theta U)+u_y\,\partial_\theta(\sin^2\theta\,f),\quad \theta\in[0,2\pi]. \tag{6}$$

The Maier-Saupe potential and Onsager potential is reduced to

$$U_{\mathrm{ms}}(\theta,t)=U_0\int_0^{2\pi}\sin^2(\theta-\theta')\,f(\theta',t)\,\mathrm{d}\theta' \tag{7}$$

$$U_{\mathrm{os}}(\theta,t)=U_0\int_0^{2\pi}|\sin(\theta-\theta')|\,f(\theta',t)\,\mathrm{d}\theta' \tag{8}$$

Design a spectral solver for system (6)-(7) and (6), (8). Depending on the choices of U_0, De and u_y, the solution will have different solutions, see [H. Yu et al., A Nonhomogeneous KineticModel of Liquid Crystal Polymers and Its Thermodynamic Closure Approximation, CiCP 2010]. Please compare the difference of using (7) and (8).

If you have enough time, try to use spherical harmonics expansion to solve system (3)-(4), but it doesn't matter if you can't finish it.

3.2 Finitely Extensible Nonlinear Elastic (FENE) Dumbbell Polymer

$$\vec{q} = \vec{x}_2 - \vec{x}_1$$

This part is about a different kind of polymer molecules. There are not rod-like, but like a soft spring. The spring force is given by

$$F(\vec{q}) = U_0 \frac{\vec{q}}{1 - |\vec{q}|^2}, \quad |\vec{q}| \leqslant 1. \tag{9}$$

where $\vec{q}$ is the vector. The corresponding potential is

$$U(\vec{q}) = -\frac{U_0}{2} \ln(1 - |\vec{q}|^2). \tag{10}$$

Let $f(\vec{q}, t)$ be the molecular probability density function, $\vec{q} \in \mathbb{R}^d$, $d = 2, 3$ and $|\vec{q}| < 1$. We also assume the molecules have indistinguishable ends, i.e. $f(\vec{q}, t) = f(-\vec{q}, t)$. The corresponding Fokker–Planck equation is given by

$$\frac{\partial f}{\partial t} = \frac{1}{\mathrm{De}} \nabla \cdot (\nabla f + f \nabla U) - \nabla \cdot (\kappa \cdot \vec{q} f), \quad \vec{q} \in \Omega := \{ \vec{q} \in \mathbb{R}^d, |\vec{q}| < 1 \} \tag{11}$$

when the definition of De, κ are same to that in equation (3).

Equation (11) is a linear equation, but have a unbounded coeffients ∇U. Design a spectral method for (3) in 2-dimensional case. The dynamics of the polymer will introduce a stress tensor to the backgound flow, which is given by

$$\tau(t) = -I + \int_\Omega \vec{q} \nabla U f(\vec{q}, t) \, \mathrm{d}\vec{q}.$$

Since (11) is a linear equation with dissipation, the solution will converge to a steady state solution, if κ is a constant. For the 2-dimensional case, numerically study how will κ affect the stress tensor in steady state.