Dissipative FE schemes for viscoelastic fluid flows

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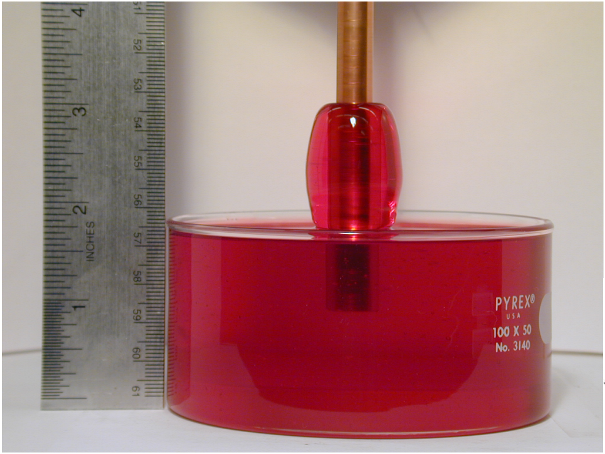
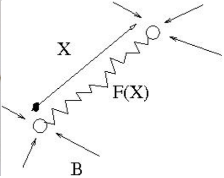
Non-standard discretizations for fluid flows, BIRS (Banff) Nov. 2010

Outline

Non-Newtonian Weissenberg effect

A viscoelastic liquid climbing along a rotating rod





Different modellings possible

- Multiscale physics: a zoo of micro-macro models.
  Langevin formalism at the scale of polymer molecules.
  Computations: expensive ! (embarrassingly parallel).
  Analysis of hybrid methods: *topic for another talk !*
- Nonlinear rheology: a zoo of constitutive laws.
  (Possibly obtained from micro-macro closures.)
  Seems more accessible for industrial applications, but
  numerical stability problems
  (e.g. at high Weissenberg numbers).

Strategy

- We have *little mathematical understanding* of constitutive ([Renardy 1985], [Guillopé Saut 1990], [Lions Masmoudi 2000], [Fernandez-CaraGuillen Ortega 2002], [Barrett Süli 2007], [Lei Liu Zhou 2008]) or micro-macro ([Lions Masmoudi 2005], [Jourdain Le bris Lelièvre 2007] [Masmoudi 2010]) models, but when sol. is smooth, **long-time asymptotics** identified ([Jourdain Le Bris Lelièvre Otto 2006]).
- **Numerical stability** of const. laws ([Owens Philips 2002]) recently improved by comput. rheologists ([Hulsen Fattal Kupferman 2005]).
- $\Rightarrow$ Can we build a **mathematical understanding** of the stability issue, **with numerical analysis tools**, based on free-energy esimates ([Jourdain Le Bris Lelièvre Otto 2006]) ?
- Numerical analyses for FD, FE, and FV schemes exist (consistency: [Baranger Machmoum 1997] [Baranger Sandri] ; stability: [Fortin Fortin] [Lozinski Owens 2003] [Lee Xu 2006]), but not for free-energy-dissipative schemes.

Outline

Mathematical setting

A Cauchy-Dirichlet problem for the Oldroyd-B model

$$
(\mathbf{P}) \begin{cases} \mathrm{Re}\left(\dfrac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) = -\nabla p + (1-\varepsilon)\Delta\boldsymbol{u} + \dfrac{\varepsilon}{\mathrm{Wi}}\,\mathrm{div}\,\boldsymbol{\sigma} \\ \mathrm{div}\,\boldsymbol{u} = 0 \\ \dfrac{\partial\boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{\sigma} = (\nabla\boldsymbol{u})\boldsymbol{\sigma} + \boldsymbol{\sigma}(\nabla\boldsymbol{u})^T - \dfrac{1}{\mathrm{Wi}}(\boldsymbol{\sigma} - \boldsymbol{I}) \end{cases}
$$

- Homogeneous Dirichlet B.C. $\boldsymbol{u} = 0$ (no flow on $\partial\mathcal{D}$) + smooth I.C. $\boldsymbol{u}(t=0) = \boldsymbol{u}_0, \boldsymbol{\sigma}(t=0) = \boldsymbol{\sigma}_0 \in \mathbb{R}^{d\times d}_{SPD}$: local-in-time regular solutions [Guillope Saut ; Fernandez–Cara Guillen Ortega]
- If global-in-time solutions still regular, unique long-time behaviour: free-energy estimate + Gromwall lemma

Free energy for the Oldroyd-B model

Link with micro-macro models (Kramers)

$$d\boldsymbol{X}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{X}_t dt = \left((\nabla\boldsymbol{u})\boldsymbol{X}_t - \frac{1}{2\mathrm{Wi}}\boldsymbol{F}(\boldsymbol{X}_t)\right)dt + \frac{1}{\sqrt{\mathrm{Wi}}}d\mathbf{B}_t$$

$$\boldsymbol{\sigma} = \frac{\varepsilon}{\mathrm{Wi}}\mathbb{E}\left[\boldsymbol{X}_t\otimes\boldsymbol{F}(\boldsymbol{X}_t)\right] = \frac{\varepsilon}{\mathrm{Wi}}\int\left[\boldsymbol{X}\otimes\boldsymbol{F}(\boldsymbol{X})\right]\psi_t(\boldsymbol{X})d\boldsymbol{X}$$

- Statistical entropy with $\boldsymbol{F}(\boldsymbol{X}) = -\nabla\ln\psi_\infty(\boldsymbol{X})$ in micro

$$F(\boldsymbol{u},\psi) = \frac{\mathrm{Re}}{2}\int_{\mathcal{D}}|\boldsymbol{u}|^2 + \frac{\varepsilon}{2\mathrm{Wi}}\int_{\mathcal{D}}\int\ln\left(\frac{\psi}{\psi_\infty}\right)\psi_\infty$$

[Jourdain Le Bris Lelièvre Otto] ARMA 181(1):97–148, 2006

- Oldroyd-B $\Leftrightarrow$ Hookean micro $\mathbf{F}(\boldsymbol{X}) = H\boldsymbol{X}$; $\psi_\infty = e^{-\frac{H}{2}|\boldsymbol{X}|^2}$

$$F(\boldsymbol{u},\boldsymbol{\sigma}) = \frac{\mathrm{Re}}{2}\int_{\mathcal{D}}|\boldsymbol{u}|^2 + \frac{\varepsilon}{2\mathrm{Wi}}\int_{\mathcal{D}}\mathrm{tr}(\boldsymbol{\sigma} - \ln\boldsymbol{\sigma} - \boldsymbol{I})$$

[Hu Lelièvre] CMS 5(4):909–916, 2007. [Boyaval Lelièvre Mangoubi] M2AN 43:523–561, 2009.

Long-time behaviour of smooth solutions

. . . at the Oldroyd-B macro level !

Test Oldroyd-B system with $(\boldsymbol{u}, \boldsymbol{I} - \boldsymbol{\sigma}^{-1})$

then $F(\boldsymbol{u}, \boldsymbol{\sigma}) = \frac{\text{Re}}{2} \int_{\mathcal{D}} |\boldsymbol{u}|^2 + \frac{\varepsilon}{2\text{Wi}} \int_{\mathcal{D}} \text{tr}(\boldsymbol{\sigma} - \ln \boldsymbol{\sigma} - \boldsymbol{I})$ satisfies

$$\frac{d}{dt} F + (1 - \varepsilon) \int_{\mathcal{D}} |\nabla \boldsymbol{u}|^2 + \frac{\varepsilon}{2\text{Wi}^2} \int_{\mathcal{D}} \text{tr}(\boldsymbol{\sigma} + \boldsymbol{\sigma}^{-1} - 2\boldsymbol{I}) = 0$$

Can we mimick that at a discrete level ? – Key points:

- $\boldsymbol{\sigma}$ must remain SPD at all times for $\boldsymbol{\sigma}^{-1}$, $\ln \boldsymbol{\sigma}$ to exist
- concavity of ln essential for $\frac{d}{dt}(\text{tr} \ln \boldsymbol{\sigma} \equiv \ln \boldsymbol{\sigma} : \boldsymbol{I}) = \frac{d\boldsymbol{\sigma}}{dt} : \boldsymbol{\sigma}^{-1}$
- transport terms $(\boldsymbol{u} \cdot \nabla)\boldsymbol{u}$ and $(\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - (\nabla \boldsymbol{u})\boldsymbol{\sigma} - \boldsymbol{\sigma}(\nabla \boldsymbol{u})^T$ must not bring spurious energy (fluid is incompressible)
- internal energy exchanges cancel by micro/macro coupling
- the remaining terms should remain dissipative

Outline

1) Time continuous – Space discrete Galerkin

Find $\boldsymbol{u}_h \in \mathrm{W}_h$, $p_h \in Q_h$, $\boldsymbol{\sigma}_h \in \mathrm{S}_h$ such that $0 \geq \ldots$:

$$0 = \mathrm{Re} \int_{\mathcal{D}} \left[\frac{\partial \boldsymbol{u}_h}{\partial t} + (\boldsymbol{u}_h \cdot \nabla) \boldsymbol{u}_h \right] \cdot \boldsymbol{u}_h$$

$$+ \int_{\mathcal{D}} \left[(1-\varepsilon) \nabla \boldsymbol{u}_h + \frac{\varepsilon}{\mathrm{Wi}} \boldsymbol{\sigma}_h \right] : \nabla \boldsymbol{u}_h$$

$$+ \frac{\varepsilon}{2\mathrm{Wi}^2} \times$$

$$0 = \mathrm{Wi} \int_{\mathcal{D}} \left[\frac{\partial \boldsymbol{\sigma}_h}{\partial t} + (\boldsymbol{u}_h \cdot \nabla) \boldsymbol{\sigma}_h - (\nabla \boldsymbol{u}_h) \boldsymbol{\sigma}_h - \boldsymbol{\sigma}_h (\nabla \boldsymbol{u}_h)^T \right] : (\boldsymbol{I} - \boldsymbol{\sigma}_h^{-1})$$

$$+ \int_{\mathcal{D}} (\boldsymbol{I} - \boldsymbol{\sigma}_h) : (\boldsymbol{I} - \boldsymbol{\sigma}_h^{-1})$$

$$\Rightarrow \boldsymbol{I}, \boldsymbol{\sigma}_h^{-1} \in \mathrm{S}_h$$

1) Time continuous – Space discrete Galerkin

Find $\boldsymbol{u}_h \in \mathrm{W}_h$, $p_h \in Q_h$, $\boldsymbol{\sigma}_h \in \mathbb{S}_h$ such that $0 \geq \ldots$:

$$0 = \mathrm{Re}\frac{d}{dt}\left(\int_{\mathcal{D}} \frac{|\boldsymbol{u}_h|^2}{2}\right) + \int_{\mathcal{D}} (\operatorname{div} \boldsymbol{u}_h)\frac{|\boldsymbol{u}_h|^2}{2}$$

$$+(1-\varepsilon)\int_{\mathcal{D}} |\boldsymbol{\nabla} \boldsymbol{u}_h|^2 + \frac{\varepsilon}{\mathrm{Wi}}\int_{\mathcal{D}} \boldsymbol{\sigma}_h : \boldsymbol{\nabla} \boldsymbol{u}_h$$

$$+\frac{\varepsilon}{2\mathrm{Wi}^2}\times$$

$$0 = \mathrm{Wi}\int_{\mathcal{D}} \left[\frac{\partial}{\partial t} + (\boldsymbol{u}_h \cdot \boldsymbol{\nabla})\right] \mathrm{tr}(\boldsymbol{\sigma}_h - \ln \boldsymbol{\sigma}_h) + \int_{\mathcal{D}} \boldsymbol{\sigma}_h : \boldsymbol{\nabla} \boldsymbol{u}_h$$

$$+\int_{\mathcal{D}} \mathrm{tr}(2\boldsymbol{I} - \boldsymbol{\sigma}_h - \boldsymbol{\sigma}_h^{-1})$$

$\Rightarrow \boldsymbol{I}, \boldsymbol{\sigma}_h^{-1} \in \mathbb{S}_h$ + $\boldsymbol{\sigma}_h \in \mathbb{R}^{d\times d}_{SPD}$ + $\mathrm{tr}(\boldsymbol{\sigma}_h - \ln \boldsymbol{\sigma}_h) \in Q_h$

1) Time continuous – Space discrete Galerkin

Find $\boldsymbol{u}_h \in \mathrm{W}_h$, $p_h \in Q_h$, $\boldsymbol{\sigma}_h \in \mathrm{S}_h$ such that $0 \geq \ldots$:

$$0 = \mathrm{Re}\frac{d}{dt}\left(\int_{\mathcal{D}} \frac{|\boldsymbol{u}_h|^2}{2}\right) + \cancel{\int_{\mathcal{D}} (\operatorname{div} \boldsymbol{u}_h)\frac{|\boldsymbol{u}_h|^2}{2}}$$

$$+(1-\varepsilon)\int_{\mathcal{D}} |\nabla \boldsymbol{u}_h|^2 + \frac{\varepsilon}{\mathrm{Wi}}\cancel{\int_{\mathcal{D}} \boldsymbol{\sigma}_h : \nabla \boldsymbol{u}_h}$$

$$+\frac{\varepsilon}{2\mathrm{Wi}^2}\times$$

$$0 = \mathrm{Wi}\int_{\mathcal{D}} \frac{\partial}{\partial t}\operatorname{tr}(\boldsymbol{\sigma}_h - \ln \boldsymbol{\sigma}_h) + \cancel{\int_{\mathcal{D}} \boldsymbol{\sigma}_h : \nabla \boldsymbol{u}_h}$$

$$+\int_{\mathcal{D}} \operatorname{tr}(2\boldsymbol{I} - \boldsymbol{\sigma}_h - \boldsymbol{\sigma}_h^{-1})$$

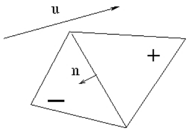
$$\mathrm{S}_h = [\mathbb{P}_0]_S^{d\times d},\ Q_h = \mathbb{P}_{d-1,disc},\ \mathrm{W}_h = [\mathbb{P}_d]^d\ (\operatorname{div} \boldsymbol{u}_h = 0)$$

1) Time continuous – Space discrete Galerkin

Consequences: we require $\boldsymbol{u}_h \cdot \boldsymbol{n}$ continuous over edges E_j,

- advection of $\boldsymbol{\sigma}_h$ requires jumps (Discontinuous Galerkin)

$$\sum_{j=1}^{N_E} \int_{E_j} |\boldsymbol{u}_h \cdot \boldsymbol{n}| [\![\boldsymbol{\sigma}_h]\!] : \{\phi\} = \sum_{j=1}^{N_E} \int_{E_j} |\boldsymbol{u}_h \cdot \boldsymbol{n}| (\boldsymbol{\sigma}_h^+ - \boldsymbol{\sigma}_h^-) : \left(\frac{\phi^+ + \phi^-}{2} \right)$$



- Scott-Vogelius velocity-pressure spaces $[\mathbb{P}_d]^d \times \mathbb{P}_{d-1,disc}$ require Arnold-Qin meshes for inf-sup stability

  NB: inf-sup stable $(\boldsymbol{u}_h, p_h)$ could also be Bernardi-Raugel $[\mathbb{P}_1]^d \oplus \{\phi_i \boldsymbol{n}_i \in \mathbb{P}_2\}_{1 \le i \le d} \times \mathbb{P}_0$ or low-order Taylor-Hood $[\mathbb{P}_2]^d \times \mathbb{P}_0$

Outline

2) Time – Space discrete Galerkin

For discretization of material time derivative of $\boldsymbol{\sigma}_h$ on $[t_n, t_{n+1}]$:

- $\frac{d}{dt}\operatorname{tr}\ln\boldsymbol{\sigma}_h = \frac{d}{dt}\boldsymbol{\sigma}_h : \boldsymbol{\sigma}_h^{-1}$ relies on the concavity of ln, which can be invoked with e.g. backward Euler + implicit testing

$$\int_{\mathcal{D}} \left(\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^{n}\right) : (\boldsymbol{\sigma}_h^{n+1})^{-1} \leq \int_{\mathcal{D}} \left(\operatorname{tr}\ln\boldsymbol{\sigma}_h^{n+1} - \operatorname{tr}\ln\boldsymbol{\sigma}_h^{n}\right)$$

- Similar trick in advection: use ln concavity + upwinding $\int_{E_j} |\boldsymbol{u}_h^n \cdot \boldsymbol{n}| [\![\boldsymbol{\sigma}_h^{n+1}]\!] : \left(\{\boldsymbol{\sigma}_h^{n+1}\} + \frac{1}{2}[\![\boldsymbol{\sigma}_h^{n+1}]\!] \equiv (\boldsymbol{\sigma}_h^{n+1})^{+\boldsymbol{u}_h}\right)$

As a result:

- the discrete free-energy estimate is only an inequality
- recall $(\nabla \boldsymbol{u}_h^{n+1})\boldsymbol{\sigma}_h^{n+1}$, the fully discrete scheme is implicit

Fully discrete numerical scheme

Find $(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{\sigma}_h^{n+1}) \in [\mathbb{P}_d]^d \times \mathbb{P}_{d-1,disc} \times [\mathbb{P}_0]_S^{d\times d} / \ \forall(\boldsymbol{v}, q, \phi)$

$$0 = \mathrm{Re}\int_{\mathcal{D}} \left[\frac{\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n}{\Delta t} + \boldsymbol{u}_h^n \cdot \nabla \boldsymbol{u}_h^{n+1} \right] \cdot \boldsymbol{v} + (1-\varepsilon)\nabla \boldsymbol{u}_h^{n+1} : \nabla \boldsymbol{v}$$

$$+ \frac{\varepsilon}{\mathrm{Wi}} \boldsymbol{\sigma}_h^{n+1} : \nabla \boldsymbol{v} - p_h^{n+1} \operatorname{div} \boldsymbol{v} + q \operatorname{div} \boldsymbol{u}_h^{n+1}$$

$$0 = \sum_{k=1}^{N_K} \int_{K_k} \left[\frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n}{\Delta t} \right] : \phi + \sum_{j=1}^{N_E} \int_{E_j} |\boldsymbol{u}_h^n \cdot \boldsymbol{n}| [\![\boldsymbol{\sigma}_h^{n+1}]\!] : \phi^+$$

$$+ \sum_{k=1}^{N_K} \int_{K_k} \left[\frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{I}}{\mathrm{Wi}} - (\nabla \boldsymbol{u}_h^{n+1})\boldsymbol{\sigma}_h^{n+1} + \boldsymbol{\sigma}_h^{n+1}(\nabla \boldsymbol{u}_h^{n+1})^T \right] : \phi$$

Discrete free-energy estimate

$$F_h^n \equiv F(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n) = \frac{\mathrm{Re}}{2}\int_{\mathcal{D}} |\boldsymbol{u}_h^n|^2 + \frac{\varepsilon}{2\mathrm{Wi}}\int_{\mathcal{D}} \mathrm{tr}(\boldsymbol{\sigma}_h^n - \ln \boldsymbol{\sigma}_h^n - \boldsymbol{I})$$

Theorem

$\forall \boldsymbol{\sigma}_h^0$ *spd*, $\exists$ *at least* 1 *discrete solution* / $\forall n \in \mathbb{N}$, $\boldsymbol{\sigma}_h^n$ *spd, and*

$$F_h^{n+1} - F_h^n + \frac{Re}{2}\int_{\mathcal{D}} |\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n|^2 + \Delta t_n(1-\varepsilon)\int_{\mathcal{D}} |\boldsymbol{\nabla} \boldsymbol{u}_h^{n+1}|^2 + \Delta t_n \frac{\varepsilon}{2Wi^2}\int_{\mathcal{D}} \mathrm{tr}\left(\boldsymbol{\sigma}_h^{n+1} + (\boldsymbol{\sigma}_h^{n+1})^{-1} - 2\boldsymbol{I}\right) \leq 0$$

Boyaval Lelièvre Mangoubi, M2AN, 43:523-561, 2009. Barrett Boyaval, M3AS, 2010, preprint arxiv:09074066

Variation 1: Advection of $\boldsymbol{\sigma}_h$

A Lagrangian approach is also possible

$$\int_{\mathcal{D}} \left[\frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n \circ \psi^n(t^n;\cdot)}{\Delta t} \right] : \boldsymbol{\phi}$$

using the flow $\psi^n(t^n;\cdot)$, but computationally more difficult

$$\left(\text{characteristics } \psi^n(t^{n+1};\boldsymbol{x}) = \boldsymbol{x}\,;\ \frac{d\psi^n(t;\boldsymbol{x})}{dt} = \boldsymbol{u}_h^n(\psi^n(t;\boldsymbol{x})) \right)$$

and even possibly unstable (depends on quadrature) !

Variation 2: Other FE spaces

- Other FE for $(\boldsymbol{u}_h, p_h)$:
  usual Navier-Stokes choices possible,
  but require vertex integration / projection in convective term
- Other (higher-degree) FE for $\boldsymbol{\sigma}_h$:
  we require disconstinuous $\pi(\boldsymbol{\sigma}_h^{-1}) \in \mathbb{P}_0$ and
  vertex integration / projection in some terms too

So higher-degree FE for $\boldsymbol{\sigma}_h$ may not be very interesting
(though full error estimation remains to be done).

NB: what about higher-order time discretization (BDF, RK) ?
(have to find corresponding test functions, nonlinear in $\boldsymbol{\sigma}_h$!)

Variation 3: Other formulations

Old history: (D)-EVSS-(G) (+ stabilization) to handle *change of type* (new entrant characteristics: OB becomes UCM).

Recently: "log-formulation" showed a bit more succesful than standard formulations by different authors ([Hulsen Fattal Kupferman 2005], [Turek]). We find quite similar constraint on discretizations.

No direct link with occurence of $\ln \sigma$ in our estimate:
only positivity preservation after discretization, see next slide.

(Lie-derivative also proposed [Lee-Xu 2006], but no numerics.)

NB: piecewise constant σ_h necessary for log: large numerical error when going back-and-forth to old/new formulations ?

Additional result 1: Uniqueness

In addition to existence of global discrete solutions which satisfies a free-energy estimate, we have uniqueness, under a CFL condition. Indeed, $\boldsymbol{\sigma}_h^{n+1}$ has to remain spd, hence:

- by Banach-Picard fixed point theorem, a solution exists within the open, convex set of spd matrices in a small ball around $\boldsymbol{\sigma}_h^n$ (for small Δt)
- by Brouwer fixed point theorem, regularized schemes (positivity constraint relaxed) have solutions, converging to a real free-energy solution after extraction of subsequence

NB: we also studied a scheme discretizing $\ln \boldsymbol{\sigma}$ rather than $\boldsymbol{\sigma}$. Then, no regularization, no subsequence, hence any solution satisfies the free-energy estimate (non spd solutions excluded).

Additional result 2: Convergence

- The free-energy dissipation implies long-time stability of discrete solutions and convergence $(\boldsymbol{u}_h^n, \boldsymbol{\sigma}_h^n) \overset{n\to\infty}{\longrightarrow} (\boldsymbol{0}, \boldsymbol{I})$ (unique stationary state: homogeneous Dirichlet BC !)
- Adding an extra-diffusion term in the Oldroyd-B equation $\Delta\boldsymbol{\sigma}$, continuous solutions to regularized discrete schemes ($\boldsymbol{\sigma}_h \in [\mathbb{P}_1]_S^{d\times d}$:trick !) can be shown to converge as $h \to 0$ to a regularized model, with truncated advection for $\boldsymbol{\sigma}$ (if $d = 2$, truncation can be replaced with a CFL condition)

[5] J.W. Barrett and S. Boyaval. Global solutions to some regularized free-energy-dissipative Oldroyd-like models (accepted for publication in M3AS), arxiv:0907.4066, 2009.

(NB: recall, accurate error estimation remains to be done)

Additional result 2 continued (some details)

To achieve free-energy-dissipative convergence with $\Delta\boldsymbol{\sigma}_h, \boldsymbol{\sigma}_h \in [\mathbb{P}_1]_S^{d\times d}$:

1. $\Delta\boldsymbol{\sigma}_h$: new BC $\boldsymbol{n}\cdot\boldsymbol{\nabla}\boldsymbol{\sigma}_h = 0$, “free-energy dissipative” on non-obtuse simplices (like for discrete maximum principle)
2. $(\boldsymbol{u}_h, p_h) \in [\mathbb{P}_2]^d \times \mathbb{P}_1$ or mini-element $[\mathbb{P}_1]^d \oplus \textit{bubble} \times \mathbb{P}_1$
3. advection $(\boldsymbol{u}_h\cdot\nabla)\boldsymbol{\sigma}_h$: discretized to avoid $\boldsymbol{\nabla}\boldsymbol{\sigma}_h$ on noting

$$\int_{\mathcal{D}} [(\boldsymbol{u}_h\cdot\nabla)\boldsymbol{\sigma}_h] : \boldsymbol{\sigma}_h^{-1} = \int_{\mathcal{D}} [(\boldsymbol{u}_h \otimes \overbrace{\boldsymbol{I}) \otimes \boldsymbol{\sigma}_h}] :: \nabla(\boldsymbol{\sigma}_h^{-1}) = \int_{\mathcal{D}} (\boldsymbol{u}_h\cdot\nabla)\ln(\boldsymbol{\sigma}_h^{-1})$$

4. vertex integration in terms $\partial_t\boldsymbol{\sigma}_h$, $\boldsymbol{\sigma}_h\boldsymbol{\nabla}\boldsymbol{u}_h$ and $\boldsymbol{I}-\boldsymbol{\sigma}_h$ to use pointwise properties of the test function $\boldsymbol{I}-\mathcal{I}_1\boldsymbol{\sigma}_h^{-1}$
5. Aubin-Lions compactness theory: quasi-uniform mesh, convex domain (test against C^0 FE projections of “$\partial_t\boldsymbol{u}_h$”). Difficulty: $\boldsymbol{\sigma}$ should remain SPD after subseq. extraction !

Extensions

. . . to other mathematical frameworks

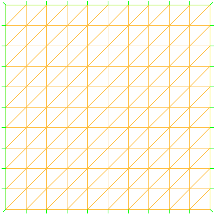
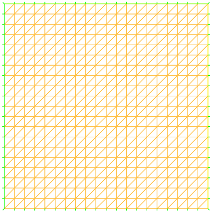
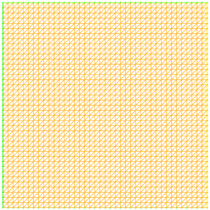
Extensions to other boundary conditions: not obvious !

But <u>other models</u> can be treated exactly the same way.

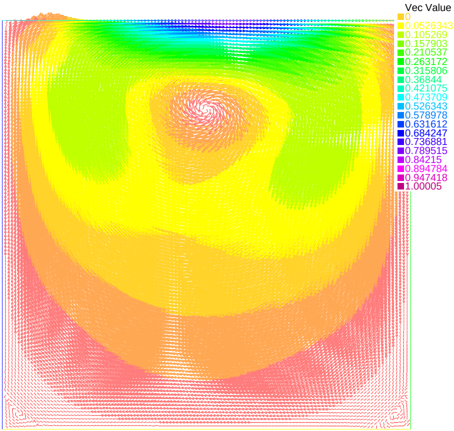
(FENE-P, debris flows: in progress, with co-authors + D. Benoît, F. Bouchut)

Lid-driven-cavity test case: setting

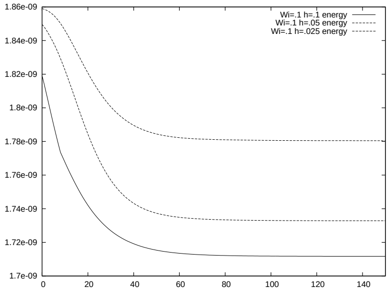
“pseudo” transient to get stationary state with
$u = [16x^2(1-x)^2, 0]$ on top, no-slip elsewhere

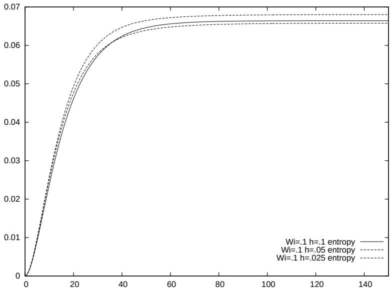




Lid-driven-cavity test case: low-Reynolds (creeping flow)

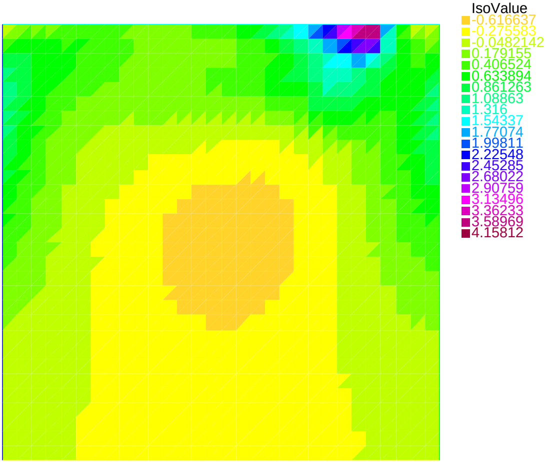


Lid-driven-cavity test case: physical quantities





Lid-driven-cavity test case: singularity



Free-energy dissipation

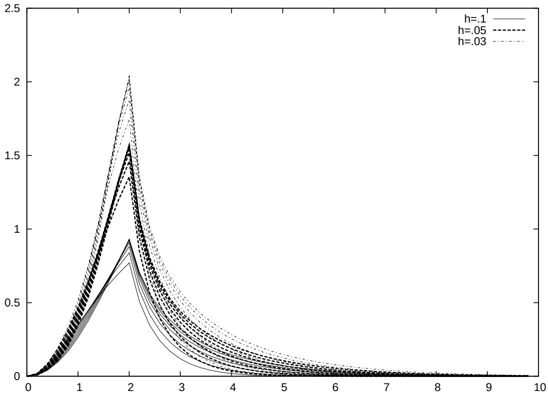


Figure: Different choices: no scheme blows up. (Anyway, no HWNP !)

Convergence: free-energy HWNP ?

Constant forcing:stationary state ?

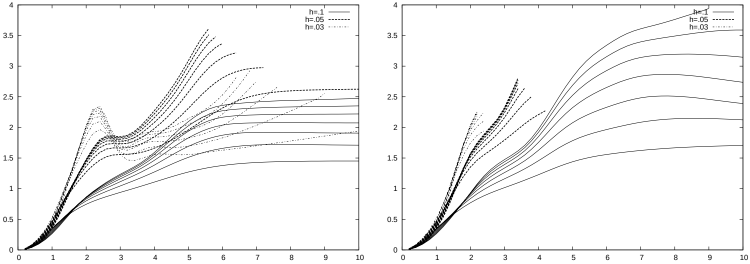
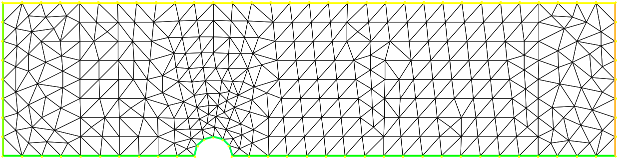


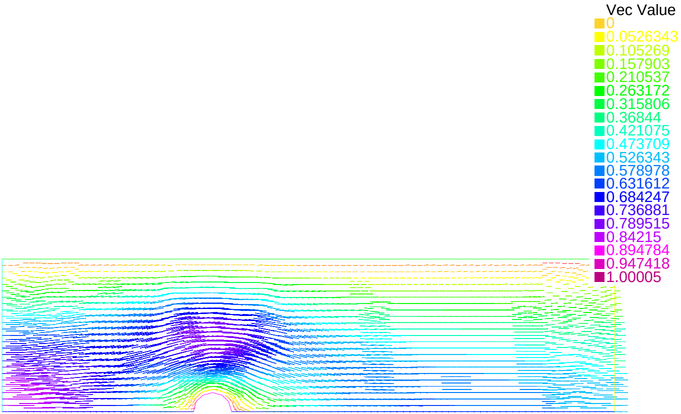
Figure: Left: $\mathbb{P}_0$ (OK) – Right: $\mathbb{P}_1$ (~~OK~~)

Flow past a cylinder test case: setting

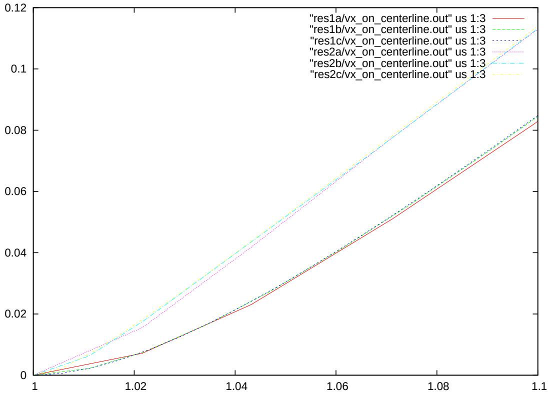
"pseudo" transient to get stationary state with inflow/outflow (perdiodic or Poiseuille + free outflow) and no-slip elsewhere



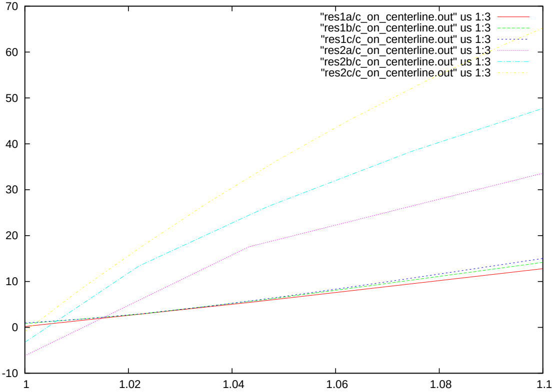
Flow past a cylinder test case: low-Reynolds (creeping flow)



Flow past a cylinder test case: velocity



Flow past a cylinder test case: stress singularity



We have shown:

- (new) physically interesting free-energy estimates (for micro-macro models and constitutive equations)
- and corresponding mathematical resuls still being explored (for discrete and continuous models).

A thorough study of numerical results wrt HWNP is still needed.

For Further Reading I

R. G. Owens and T. N. Philips.
Computational rheology.
Imperial College Press / World Scientific, 2002.

B. Jourdain, C. Le Bris, T. Lelièvre, and F. Otto.
Long-time asymptotics of a multiscale model for polymeric fluid flows.
Archive for Rational Mechanics and Analysis, 181(1):97–148, 2006.

D. Hu and T. Lelièvre.
New entropy estimates for the Oldroyd-B model, and related models.
Commun. Math. Sci., 5(4):906–916, 2007.

For Further Reading II

S. B., T. Lelièvre and C. Mangoubi
Free-energy-dissipative schemes for the Oldroyd-B model
M2AN, 43 : 523-561, 2009.

J. W. Barrett and S. B.
Existence and approximation of a (regularized) Oldroyd-B model.
(Accepted for publication in M3AS, preprint http://fr.arxiv.org/abs/0907.4066) 2010.

Parametrized r.v. $Z^\mu \in L^2(\Omega)$ in Monte-Carlo

Goal: compute expectation $E(Z^\mu)$ for many μ.

Monte-Carlo with confidence intervals (CLT+Slutsky) $\forall a > 0$

$$\mathrm{E}_M(Z^\mu) := \frac{1}{M}\sum_{m=1}^{M} Z_m^\mu \xrightarrow[M\to\infty]{P-a.s.} E(Z^\mu) \qquad \mathrm{Var}_M(Z^\mu) = \dots$$

$$P\left(|\mathrm{E}_M(Z^\mu) - E(Z^\mu)| \leq a\sqrt{\frac{\mathrm{Var}_M(Z^\mu)}{M}}\right) \xrightarrow[M\to\infty]{} \int_{-a}^{a} \frac{e^{-x^2/2}}{\sqrt{2\pi}}dx$$

Faster MC with variance reduced by control variates Y^μ:

Compute $E(Z^\mu) = E(Z^\mu - Y^\mu) + E(Y^\mu)$ where

- $E(Y^\mu)$ is known (here $E(Y^\mu) = 0$)
- $Var(Z^\mu) \geq Var(Z^\mu - Y^\mu)$.

Control variates: practical variance reduction

Ideally $Y^\mu = Z^\mu - E(Z^\mu) \Rightarrow Var(Z^\mu - Y^\mu) = 0$, but in practice:

Compute $\tilde{Y}^\mu \approx Y^\mu$ minimizing

$$Var(Z^\mu - \tilde{Y}^\mu) = E\left(\left|(Z^\mu - E(Z^\mu)) - \tilde{Y}^\mu\right|^2\right) = E\left(\left|Y^\mu - \tilde{Y}^\mu\right|^2\right)$$

Faster MC with RB approach :

$$\tilde{Y}^\mu := \sum_{n=1}^{N} \alpha_n(\mu) Y^{\mu_n} = \sum_{n=1}^{N} \alpha_n(\mu) \left(Z^{\mu_n} - E(Z^{\mu_n})\right)$$

where the $\alpha_n(\mu)$ minimize $Var(Z^\mu - \tilde{Y}^\mu)$

$$\mathrm{E}_{\mathrm{M_{small}}}\left(Z^\mu - \tilde{Y}^\mu\right) = \frac{1}{\mathrm{M_{small}}} \sum_{m=1}^{\mathrm{M_{small}}} (Z^\mu_m - \tilde{Y}^\mu_m) \xrightarrow[\mathrm{M_{small}} \to \infty]{P-a.s.} E(Z^\mu).$$

Control variates: practical variance reduction

Ideally $Y^\mu = Z^\mu - E(Z^\mu) \Rightarrow Var(Z^\mu - Y^\mu) = 0$, but in practice:

Compute $\tilde{Y}^\mu \approx Y^\mu$ minimizing

$$Var(Z^\mu - \tilde{Y}^\mu) = E\left(\left|(Z^\mu - E(Z^\mu)) - \tilde{Y}^\mu\right|^2\right) = E\left(\left|Y^\mu - \tilde{Y}^\mu\right|^2\right)$$

Faster MC with RB approach :

$$\tilde{Y}^\mu := \sum_{n=1}^{N} \alpha_n(\mu) Y^{\mu_n} \approx \sum_{n=1}^{N} \alpha_n(\mu) \left(Z^{\mu_n} - \mathrm{E}_{\mathrm{M}_{\mathrm{large}}}(Z^{\mu_n})\right)$$

where the $\alpha_n(\mu)$ minimize $\mathrm{Var}_{\mathrm{M}_{\mathrm{small}}}(Z^\mu - \tilde{Y}^\mu)$

$$\mathrm{E}_{\mathrm{M}_{\mathrm{small}}}\left(Z^\mu - \tilde{Y}^\mu\right) = \frac{1}{\mathrm{M}_{\mathrm{small}}} \sum_{m=1}^{\mathrm{M}_{\mathrm{small}}} (Z^\mu_m - \tilde{Y}^\mu_m) \xrightarrow[\mathrm{M}_{\mathrm{small}}\to\infty]{P-a.s.} E(Z^\mu).$$

Effective RB control variates method in practice

Effective numerical variance minimizations:

For all μ, solve the least-square problem by usual methods

$$\inf_{\{\alpha_1(\mu),\dots,\alpha_N(\mu)\}} \mathrm{Var}_{\mathrm{M}_{\mathrm{small}}} \left(Z^\mu - \sum_{n=1}^{N} \alpha_n(\mu) \left(Z^{\mu_n} - E(Z^{\mu_n}) \right) \right)$$

For instance, SVD or QR for the normal equations ($i = 1, \dots, N$)
$\sum_{j=1}^{N} \mathrm{Cov}_{\mathrm{M}_{\mathrm{small}}} \left(Z^{\mu_i}, Z^{\mu_j} \right) \alpha_j^\mu = \mathrm{Cov}_{\mathrm{M}_{\mathrm{small}}} \left(Z^{\mu_i}, Z^\mu \right)$

Computational gains:

Only in the many-query limit = many μ !
(Offline: N expensive computations $\mathrm{E}_{\mathrm{M}_{\mathrm{large}}}(Z^{\mu_n})$ + greedy)
$\Rightarrow$ OK for many observations $s^\star$, or a large response surface !