Thermodynamics of fluids: Analysis and/or numerics

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Navier-Stokes-Fourier system

Mass conservation

$$\partial_t \varrho + \mathrm{div}_x(\varrho \mathbf{u}) = 0$$

Momentum balance

$$\partial_t(\varrho \mathbf{u}) + \mathrm{div}_x(\varrho \mathbf{u} \otimes \mathbf{u}) + \nabla_x p(\varrho, \vartheta) = \mathrm{div}_x \mathbb{S}(\nabla_x \mathbf{u})$$

$$\mathrm{div}_x \mathbb{S}(\nabla_x \mathbf{u}) \equiv \mu \Delta \mathbf{u} + \lambda \nabla_x \mathrm{div}_x \mathbf{u}, \ \ \mu > 0, \ \ \lambda \geq 0$$

Internal energy equation

$$c_v \left[\partial_t(\varrho \vartheta) + \mathrm{div}_x(\vartheta \mathbf{u}) \right] - \mathrm{div}_x \left(\kappa(\vartheta) \nabla_x \vartheta \right)$$

$$= \mathbb{S}(\nabla_x \mathbf{u}) : \nabla_x \mathbf{u} - p_\vartheta(\varrho, \vartheta) \mathrm{div}_x \mathbf{u}, \ \ \kappa(\vartheta) > 0$$

Initial and boundary conditions

$\varrho(0, \cdot) = \varrho_0 > 0, \ \vartheta(0, \cdot) = \vartheta_0 > 0, \ \mathbf{u}(0, \cdot) = \mathbf{u}_0,$ spatially periodic b.c.

Analytical approximation

Mass conservation

$$\partial_t \varrho + \mathrm{div}_x(\varrho \mathbf{u}) = \varepsilon \boxed{\Delta_x \varrho}$$

Momentum balance

$$\partial_t(\varrho \mathbf{u}) + \mathrm{div}_x(\varrho \mathbf{u} \otimes \mathbf{u}) + \nabla_x p(\varrho, \vartheta) = \mathrm{div}_x \mathbb{S}(\nabla_x \mathbf{u})$$

$$-\varepsilon \boxed{\nabla_x \mathbf{u} \nabla_x \varrho}$$

Internal energy equation

$$c_v \left[\partial_t(\varrho \vartheta) + \mathrm{div}_x(\vartheta \mathbf{u})\right] - \mathrm{div}_x \left(\kappa(\vartheta) \nabla_x \vartheta\right)$$

$$= \mathbb{S}(\nabla_x \mathbf{u}) : \nabla_x \mathbf{u} - p_\vartheta(\varrho, \vartheta) \mathrm{div}_x \mathbf{u}, \ \ \kappa(\vartheta) > 0$$

Total energy balance

Pressure

$$p(\varrho, \vartheta) = a\varrho^{\gamma} + b\varrho + \varrho\vartheta, \ \ \gamma > 3, \ \ a, b > 0$$

Total energy balance

$$E(t) = \int \left[\frac{1}{2}\varrho|\mathbf{u}|^2 + c_v\varrho\vartheta + \frac{a}{\gamma - 1}\varrho^{\gamma} + b\varrho \log(\varrho) \right]$$

$$\frac{\mathrm{d}}{\mathrm{d}t} E(t) = 0$$

Numerical solution

FV framework

$$\text{regular tetrahedral mesh}, \ Q_h = \{ v \mid v = \text{piece-wise constant} \}$$

FE framework - Crouzeix - Raviart

$$V_h = \left\{ v \ \middle| \ v = \text{piece-wise affine}, \ \tilde{v}_\Gamma \text{ continuous on face } \Gamma \right\}$$

$$\tilde{v}_\Gamma \equiv \frac{1}{|\Gamma|} \int_\Gamma v \ \mathrm{dS}_x$$

Upwind discretization of convective terms

$$\langle h\mathbf{u}; \nabla_x \varphi \rangle_E \approx \sum_\Gamma \int_\Gamma h(\cdot - \tilde{\mathbf{u}}_\Gamma \cdot \mathbf{n}) \tilde{\mathbf{u}}_\Gamma \cdot \mathbf{n} [[\varphi]] \ \mathrm{dS}_x$$

$$\equiv \sum_\Gamma \int_\Gamma \mathrm{Up}[h, \mathbf{u}] [[\varphi]] \ \mathrm{dS}_x$$

Numerical scheme [Karlsen-Karper], I

Equation of continuity

$$\int_\Omega D_t \varrho_h^k \varphi_h \,\mathrm{d}x \equiv \int_\Omega \frac{\varrho_h^k - \varrho_h^{k-1}}{\Delta t} \varphi_h \,\mathrm{d}x = \sum_{\Gamma \in \Gamma_h} \int_\Gamma \mathrm{Up}[\varrho_h^k, u_h^k] \, [[\varphi_h]] \,\mathrm{dS}_x$$

$$-h^\alpha \boxed{\sum_{\Gamma \in \Gamma_h} \int_\Gamma [[\varrho_h^k]][[\varphi_h]] \,\mathrm{dS}_x} \text{ for all } \varphi_h \in Q_h$$

Numerical scheme [Karlsen-Karper], II

Momentum equation

$$\int_\Omega D_t\left(\varrho_h^k \widehat{\mathbf{u}}_h^k\right) \cdot \varphi_h \ \mathrm{d}x - \sum_{\Gamma \in \Gamma_h} \int_\Gamma \mathrm{Up}[\varrho_h^k \widehat{\mathbf{u}}_h^k, \mathbf{u}_h^k] \ \cdot [[\widehat{\varphi}_h]] \mathrm{dS}_x$$

$$- \int_\Omega p(\varrho_h^k, \vartheta_h^k) \mathrm{div}_x \varphi_h \ \mathrm{d}x - h^\alpha \boxed{\sum_{\Gamma \in \Gamma_h} \int_\Gamma [[\varrho_h^k]][[\widehat{\varphi}_h]] \left\{\widehat{\mathbf{u}}_h^k\right\} \mathrm{dS}_x}$$

$$= - \int_\Omega \left(\mu \nabla_h \mathbf{u}_h : \nabla_h \varphi + \lambda \mathrm{div}_h \mathbf{u}_h^k \mathrm{div}_h \varphi_h\right) \ \mathrm{d}x$$

for all $\varphi_h \in V_h(\Omega)$

Numerical scheme [Karlsen-Karper], III

Energy equation

$$\int_\Omega D_t \left(\varrho_h^k \vartheta_h^k\right) \varphi_h \, \mathrm{d}x - \sum_{\Gamma \in \Gamma_h} \int_\Gamma \mathrm{Up}[\varrho_h^k \vartheta_h^k, \mathbf{u}_h^k] \, [[\varphi_h]] \mathrm{d}S_x$$

$$+ \sum_{\Gamma \in \Gamma_h} \int_\Gamma \frac{1}{d_h} [[K(\vartheta_h^k)]] \, [[\varphi_h]] \mathrm{d}S_x$$

$$= \int_\Omega \left(\mu |\nabla_h \mathbf{u}_h^k|^2 + \lambda |\mathrm{div}_h \mathbf{u}_h^k|^2\right) \varphi_h \, \mathrm{d}x$$

$$- \int_\Omega \vartheta_h^k \partial_\vartheta p(\varrho_h^k, \vartheta_h^k) \mathrm{div}_x \mathbf{u}_h^k \varphi_h \, \mathrm{d}x$$

for all $\varphi_h \in Q_h(\Omega)$

Frequently asked questions...

Analysis

- Are there *a priori* bounds for solutions?
- Does the problem admit a solution and in which sense?
- Is the solution unique and regular?

Numerics

- Is the numerical method stable?
- Is the numerical method convergent?
- Is the convergence unconditional; what are the error estimates?

Convergence of bounded solutions

Suppose that the numerical solutions remain bounded for $h \to 0$. Do they converge? And to what?

Do we need analysis?

An example - variable density flow in porous media

$$\partial_t \varrho + \mathrm{div}_x(\varrho \mathbf{u}) = 0$$

$$\partial_t(\varrho c(\varrho)) + \mathrm{div}_x(\varrho c(\varrho)\mathbf{u}) - \mathrm{div}_x(\varrho D \nabla_x c(\varrho)) = 0$$

$$\mathbf{u} = \nabla_x p - \varrho \mathbf{g}$$

Compatibility

$$c = \log(\varrho) \ \Rightarrow \Delta p = \Delta \varrho + |\nabla_x \log(\varrho)|^2 + \mathrm{div}_x(\varrho \mathbf{g})$$

periodic boundary conditions $\Rightarrow$ $\varrho = \mathrm{const}$!

Navier-Stokes-Fourier system (weak form)

Mass conservation

$$\partial_t \varrho + \mathrm{div}_x(\varrho \mathbf{u}) = 0$$

Momentum balance

$$\partial_t(\varrho \mathbf{u}) + \mathrm{div}_x(\varrho \mathbf{u} \otimes \mathbf{u}) + \nabla_x p(\varrho, \vartheta) = \mathrm{div}_x \mathbb{S}(\nabla_x \mathbf{u})$$

Thermal energy balance

$$c_v \partial_t(\varrho\vartheta) + c_v \mathrm{div}_x(\varrho\vartheta\mathbf{u}) - \Delta(\overline{K(\vartheta)})$$

$$\boxed{\geq} \mathbb{S}(\nabla_x \mathbf{u}) : \nabla_x \mathbf{u} - p_\vartheta(\varrho, \vartheta)\vartheta \mathrm{div}_x \mathbf{u}, \ \ \varrho\overline{K(\vartheta)} = \varrho K(\vartheta)$$

Total energy balance

$$\int \left[\frac{1}{2}\varrho|\mathbf{u}|^2 + \frac{a}{\gamma - 1}\varrho^\gamma + b\varrho \log(\varrho) + c_v \varrho\vartheta \right] (\tau, \cdot) \ \mathrm{d}x \boxed{\leq} E_0$$

Existence vs. convergence

Existence of weak solutions [E.F.2003]

The Navier-Stokes-Fourier system admits a global-in-time weak solution for any finite energy initial data

Convergence of the numerical scheme [E.F., T.Karper, A.Novotný 2014]

The numerical solutions converge, up to a subsequence, to a weak solution of the Navier-Stokes-Fourier system

Blow-up criterion

Blow-up of smooth solutions [E.F., Y.Sun 2014]

Suppose that the initial data ϱ_0, ϑ_0, and $\mathbf{u}_0$ are smooth ($W^{2,3}$). Then the Navier-Stokes-Fourier system admits a strong solution defined on a (possibly short) time interval $(0, T)$.
If

$$\sup_{t \in (0,T)} \left[\|\varrho\|_{L^\infty} + \|\vartheta\|_{L^\infty} + \|\mathbf{u}\|_{L^\infty} \right] < \infty,$$

then the solution can be extended beyond T.

Regularity criterion

Regularity for weak solutions [E.F., Y.Sun 2014]

Suppose that the initial data ϱ_0, ϑ_0, and $\mathbf{u}_0$ are smooth ($W^{2,3}$). Let $[\varrho, \vartheta, \mathbf{u}]$ be a weak solution of the Navier-Stokes-Fourier system such that

$$\sup_{t \in (0,T)} \left[\|\varrho\|_{L^\infty} + \|\vartheta\|_{L^\infty} + \|\mathbf{u}\|_{L^\infty} + \|\mathrm{div}_x \mathbf{u}\|_{L^\infty} \right] < \infty.$$

Then $[\varrho, \vartheta, \mathbf{u}]$ is regular.

Synergy analysis - numerics, assumptions

Numerical solutions with regular initial data

Suppose that $[\varrho_h, \vartheta_h, \mathbf{u}_h]$ is a sequence of numerical solutions for regular initial data

Boundedness

Suppose that

$$\varrho_h^k, \ \vartheta_h^k, \ \mathbf{u}_h^k, \ \mathrm{div}_h \mathbf{u}_h^k$$

are bounded independently of the order of discretization h.

Synergy analysis - numerics, conclusion

Conclusion

The numerical solutions converge to a weak solution with

$$\sup_{t\in(0,T)} \left[\|\varrho\|_{L^\infty} + \|\vartheta\|_{L^\infty} + \|\mathbf{u}\|_{L^\infty} + \|\mathrm{div}_x \mathbf{u}\|_{L^\infty} \right] < \infty.$$

Consequently:

- the limit solution is smooth
- the limit solution is unique
- the numerical scheme converges unconditionally
- error estimates (?)