Kinetic Derivation and Existence of Strong Solutions for Diffuse Interface Fluid Models

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France-Korea IRL webinar in PDE December 16th 2022

Supported by grant ANR-19-CE05-0037-02 of Agence Nationale de la Recherche

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2 Diffuse Interface Fluids

Diffuse Interface Models from Thermodynamics

- **Diffuse interface fluids from thermodynamics**

  Van der Waals (1891)   Korteweg (1901)   Dunn and Serrin (1985)

- **Cahn-Hilliard fluids from thermodynamics**

  Cahn and Hilliard (1958) (1959)   Lowengrub and Truskinovsky (1997)
  Falk (1992)   Verschueren (1999)   Heida et al. (2012)

- **Ambiguity of thermodynamic derivations from kinetic derivation**

  Giovangigli (2020) (2021)

Diffuse Interface Fluids (1)

- **Van der Waals free energy and thermodynamic functions**

$$\mathcal{A} = \mathcal{A}^{\mathrm{cl}}(\rho, T) + \tfrac{1}{2}\varkappa|\boldsymbol{\nabla}\rho|^2 \qquad \mathcal{S} = \mathcal{S}^{\mathrm{cl}}(\rho, T) - \tfrac{1}{2}\partial_T\varkappa|\boldsymbol{\nabla}\rho|^2 \qquad g = g^{\mathrm{cl}}(\rho, T)$$

$$\mathcal{E} = \mathcal{E}^{\mathrm{cl}}(\rho, T) + \tfrac{1}{2}(\varkappa - T\partial_T\varkappa)|\boldsymbol{\nabla}\rho|^2 \qquad p = p^{\mathrm{cl}}(\rho, T) - \tfrac{1}{2}\varkappa|\boldsymbol{\nabla}\rho|^2$$

Gibbs relation $\quad T\, d\mathcal{S} = \, d\mathcal{E} - g\, d\rho - \varkappa\boldsymbol{\nabla}\rho\boldsymbol{\cdot}\, d\boldsymbol{\nabla}\rho$

- **Conservation equations**

$$\partial_t\rho + \boldsymbol{\nabla\cdot}(\rho\boldsymbol{v}) = 0$$

$$\partial_t(\rho\boldsymbol{v}) + \boldsymbol{\nabla\cdot}(\rho\boldsymbol{v}\otimes\boldsymbol{v}) + \boldsymbol{\nabla\cdot}\boldsymbol{\mathcal{P}} = 0$$

$$\partial_t\big(\mathcal{E} + \tfrac{1}{2}\rho|\boldsymbol{v}|^2\big) + \boldsymbol{\nabla\cdot}\Big(\boldsymbol{v}\big(\mathcal{E} + \tfrac{1}{2}\rho|\boldsymbol{v}|^2\big)\Big) + \boldsymbol{\nabla\cdot}(\boldsymbol{\mathcal{Q}} + \boldsymbol{\mathcal{P}}\boldsymbol{\cdot}\boldsymbol{v}) = 0$$

Diffuse Interface Fluids (2)

- **Transport fluxes**

$$\boldsymbol{\mathcal{P}} = p\boldsymbol{I} + \varkappa \boldsymbol{\nabla}\rho \otimes \boldsymbol{\nabla}\rho - \rho \boldsymbol{\nabla}\cdot(\varkappa \boldsymbol{\nabla}\rho)\boldsymbol{I} + \boldsymbol{\mathcal{P}}^{\mathrm{d}}$$

$$\boldsymbol{\mathcal{Q}} = \varkappa \rho \boldsymbol{\nabla}\cdot\boldsymbol{v}\, \boldsymbol{\nabla}\rho + \boldsymbol{\mathcal{Q}}^{\mathrm{d}}$$

$$\boldsymbol{\mathcal{P}}^{\mathrm{d}} = -\,\mathfrak{v}\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\boldsymbol{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^t - \tfrac{2}{d}\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\boldsymbol{I}\big) \qquad \boldsymbol{\mathcal{Q}}^{\mathrm{d}} = -\lambda\boldsymbol{\nabla}T$$

- **Entropy balance**

$$\partial_t \mathcal{S} + \boldsymbol{\nabla}\cdot(\boldsymbol{v}\mathcal{S}) + \boldsymbol{\nabla}\cdot\left(\frac{\boldsymbol{\mathcal{Q}}}{T} - \frac{\varkappa\rho\boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla}\rho}{T}\right)$$

$$= -\frac{1}{T}\Big(\boldsymbol{\mathcal{P}} - p\boldsymbol{I} - \varkappa\boldsymbol{\nabla}\rho\otimes\boldsymbol{\nabla}\rho + \rho\boldsymbol{\nabla}\cdot(\varkappa\boldsymbol{\nabla}\rho)\,\boldsymbol{I}\Big):\boldsymbol{\nabla}\boldsymbol{v} - \Big(\boldsymbol{\mathcal{Q}} - \varkappa\rho\boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla}\rho\Big)\cdot\boldsymbol{\nabla}\Big(\frac{-1}{T}\Big)$$

$$= \frac{\lambda}{T^2}|\boldsymbol{\nabla}T|^2 + \frac{\mathfrak{v}}{T}(\boldsymbol{\nabla}\cdot\boldsymbol{v})^2 + \frac{\eta}{2T}\Big|\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^t - \tfrac{2}{d}\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\boldsymbol{I}\Big|^2$$

Diffuse Interface Fluids (3)

- **Thermodynamic stability**

  Assume that $\mathsf{z}^{\rm cl} = (\rho, T)^t \;\mapsto\; \mathsf{u}^{\rm cl} = (\rho, \mathcal{E}^{\rm cl})^t$ is locally invertible then

$$\partial^2_{\mathsf{u}^{\rm cl}\mathsf{u}^{\rm cl}} \mathcal{S}^{\rm cl} \;\text{ negative definite } \iff \partial_T \mathcal{E}^{\rm cl} > 0 \text{ and } \partial_\rho p^{\rm cl} > 0$$

- **Assumptions on thermodynamics**

($\mathsf{H}^{\rm cl}_1$) *$\mathcal{E}^{\rm cl}$, $p^{\rm cl}$, and $\mathcal{S}^{\rm cl}$ are C^γ functions of $\mathsf{z}^{\rm cl} = (\rho, T)^t$ over $\mathcal{O}_{\mathsf{z}^{\rm cl}}$*
$\mathcal{O}_{\mathsf{z}^{\rm cl}} \subset (0,\infty)^2$ simply connected nonempty open set.

($\mathsf{H}^{\rm cl}_2$) *Letting $\mathcal{G}^{\rm cl} = \mathcal{E}^{\rm cl} + p^{\rm cl} - T\mathcal{S}^{\rm cl} = \rho g^{\rm cl}$ then $T\, d\mathcal{S}^{\rm cl} = d\mathcal{E}^{\rm cl} - g^{\rm cl}\, d\rho$*

($\mathsf{H}^{\rm cl}_3$) *$\mathcal{O}_{\mathsf{z}^{\rm cl}}$ is increasing with T and $\partial_T \mathcal{E}^{\rm cl} > 0$*

3 Kinetic Derivation

Kinetic Theory and Interfaces

- **Vlasov equations or linearized Boltzmann with condensation**

  de Sobrino (1967) Grmela (1971) Karkhek and Stell (1981) Aoki et al. (1990) Cercignani (2000) Frezzotti (2005) (2011)

- **Equilibrium statistical mechanics**

  Kirkwood and Buff (1949) Ono and Kondo (1960) Evans (1979) Davis and Scriven (1982) Rowlinson and Widom (1989)

- **Kinetic theory and diffuse interface models**

  Rocard (1933) Piechór (2008) Takata et al. (2018) (2021) Giovangigli (2020) (2021)

Kinetic framework (1)

- **BBGKY hierarchy**

  $f_1(\mathbf{r}_1, \boldsymbol{c}_1, t)$ one-particle distribution $\quad f_2(\mathbf{r}_1, \boldsymbol{c}_1, \mathbf{r}_2, \boldsymbol{c}_2, t)$ pair distribution

  $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1 \quad r_{12} = |\mathbf{r}_{12}|$

$$\partial_t f_1 + \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} f_1 = \int \theta_{12} f_2 \, d\mathbf{r}_2 \, d\boldsymbol{c}_2$$

$$\partial_t f_2 + \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} f_2 + \boldsymbol{c}_2 \cdot \boldsymbol{\nabla}_{\mathbf{r}_2} f_2 - \theta_{12} f_2 = \int (\theta_{13} + \theta_{23}) f_3 \, d\mathbf{r}_3 \, d\boldsymbol{c}_3$$

- **Operator $\boldsymbol{\theta_{12}}$**

  m mass of a particle $\quad \varphi = \varphi(r_{12})$ pair interaction potential

$$\theta_{12} = \frac{1}{m} \boldsymbol{\nabla}_{\mathbf{r}_1} \varphi \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_1} + \frac{1}{m} \boldsymbol{\nabla}_{\mathbf{r}_2} \varphi \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_2}$$

Kinetic framework (2)

- **Cluster expansion of pair distributions**

$$\mathfrak{S}_{12} = \exp\left(-t\mathfrak{H}_{12}\right)\exp\left(t\mathfrak{H}_{1}\right)\exp\left(t\mathfrak{H}_{2}\right) \qquad \text{Neglect triple collisions}$$

$$\mathfrak{H}_1 = \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} \qquad \mathfrak{H}_{12} = \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} + \boldsymbol{c}_2 \cdot \boldsymbol{\nabla}_{\mathbf{r}_2} - \theta_{12}$$

$$f_2(\mathbf{r}_1, \boldsymbol{c}_1, \mathbf{r}_2, \boldsymbol{c}_2, 0) = f_1(\mathbf{r}_1, \boldsymbol{c}_1, 0) f_1(\mathbf{r}_2, \boldsymbol{c}_2, 0) \qquad f_2 = \mathfrak{S}_{12} f_1(\mathbf{r}_1, \boldsymbol{c}_1, t) f_1(\mathbf{r}_2, \boldsymbol{c}_2, t)$$

$$\tau_{12}(\mathbf{r}_1, \boldsymbol{c}_1, \mathbf{r}_2, \boldsymbol{c}_2) = \lim_{t \to \infty} \mathfrak{S}_{12}(\mathbf{r}_1, \boldsymbol{c}_1, \mathbf{r}_2, \boldsymbol{c}_2, t)$$

- **Generalized Boltzmann equations**

$$\partial_t f_1 + \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} f_1 = \mathcal{J}(f_1) = \int \theta_{12} \tau_{12} f_1(\mathbf{r}_1, \boldsymbol{c}_1, t) f_1(\mathbf{r}_2, \boldsymbol{c}_2, t)\, d\mathbf{r}_2\, d\boldsymbol{c}_2$$

Kinetic framework (3)

- **Action of the streaming operator**

$$(\mathbf{r}_1', \boldsymbol{c}_1', \mathbf{r}_2', \boldsymbol{c}_2') = \tau_{12}(\mathbf{r}_1, \boldsymbol{c}_1, \mathbf{r}_2, \boldsymbol{c}_2)$$

$$m\boldsymbol{c}_1 + m\boldsymbol{c}_2 = m\boldsymbol{c}_1' + m\boldsymbol{c}_2' \qquad m\mathbf{r}_1 + m\mathbf{r}_2 = m\mathbf{r}_1' + m\mathbf{r}_2'$$

$$\tfrac{1}{2}m|\boldsymbol{c}_1|^2 + \tfrac{1}{2}m|\boldsymbol{c}_2|^2 + \varphi(r_{12}) = \tfrac{1}{2}m|\boldsymbol{c}_1'|^2 + \tfrac{1}{2}m|\boldsymbol{c}_2'|^2$$

- **Bogoliubov distribution**

$$f_2(\mathbf{r}_1, \boldsymbol{c}_1, \mathbf{r}_2, \boldsymbol{c}_2, t) = \tau_{12} f_1(\mathbf{r}_1, \boldsymbol{c}_1, t) f_1(\mathbf{r}_2, \boldsymbol{c}_2, t) = f_1(\mathbf{r}_1', \boldsymbol{c}_1', t)\, f_1(\mathbf{r}_2', \boldsymbol{c}_2', t)$$

- **Decomposition of f_2**

$$f_2 = f_1(\mathbf{r}_1, \boldsymbol{c}_1', t)\, f_1(\mathbf{r}_1, \boldsymbol{c}_2', t) + \big(f_1(\mathbf{r}_1', \boldsymbol{c}_1', t)\, f_1(\mathbf{r}_2', \boldsymbol{c}_2', t) - f_1(\mathbf{r}_1, \boldsymbol{c}_1', t)\, f_1(\mathbf{r}_1, \boldsymbol{c}_2', t)\big)$$

Kinetic framework (4)

- **Decomposition of $\mathcal{J} = \mathcal{J}^{(0)} + \mathcal{J}^{(1)}$**

$$\mathcal{J}^{(0)}(f_1) = \int \theta_{12} f_1(\mathbf{r}_1, \boldsymbol{c}_1', t) f_1(\mathbf{r}_1, \boldsymbol{c}_2', t)\, d\mathbf{r}_2\, d\boldsymbol{c}_2$$

$$\mathcal{J}^{(1)}(f_1) = \int \theta_{12} \big(f_1(\mathbf{r}_1', \boldsymbol{c}_1', t) f_1(\mathbf{r}_2', \boldsymbol{c}_2', t) - f_1(\mathbf{r}_1, \boldsymbol{c}_1', t) f_1(\mathbf{r}_1, \boldsymbol{c}_2', t) \big)\, d\mathbf{r}_2\, d\boldsymbol{c}_2$$

$\mathcal{J}^{(0)}(f)$ coincide with Boltzmann collision operator

- **Generalized Boltzmann equation**

$$\partial_t f_1 + \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} f_1 = \mathcal{J}^{(0)}(f_1) + \mathcal{J}^{(1)}(f_1)$$

Kinetic framework (5)

- **Number densities and fluid velocity**

$$n(\mathbf{r},t) = \int f_1(\mathbf{r},\boldsymbol{c}_1,t)\,d\boldsymbol{c}_1 \qquad \rho = mn$$

$$\rho(\mathbf{r},t)\,\boldsymbol{v}(\mathbf{r},t) = \int m\boldsymbol{c}_1 f_1(\mathbf{r},\boldsymbol{c}_1,t)\,d\boldsymbol{c}_1 \qquad \mathbf{r} = \mathbf{r}_1$$

- **Internal energy**

$$\mathcal{E} = \mathcal{E}^{\mathrm{K}} + \mathcal{E}^{\mathrm{P}} \qquad \mathcal{E}^{\mathrm{K}}(\mathbf{r},t) = \int \tfrac{1}{2}m|\boldsymbol{c}_1 - \boldsymbol{v}|^2 f_1(\mathbf{r},\boldsymbol{c}_1,t)\mathrm{d}\boldsymbol{c}_1$$

$$\mathcal{E}^{\mathrm{P}}(\mathbf{r},t) = \int \tfrac{1}{2}\varphi(r_{12})n_{12}(\mathbf{r},\mathbf{r}+\mathbf{r}_{12},t)\mathrm{d}\mathbf{r}_{12}$$

$$n_{12}(\mathbf{r}_1,\mathbf{r}_2,t) = \int f_2(\mathbf{r}_1,\boldsymbol{c}_1,\mathbf{r}_2,\boldsymbol{c}_2,t)\mathrm{d}\boldsymbol{c}_1\mathrm{d}\boldsymbol{c}_2 \qquad \mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$$

Kinetic framework (6)

- **Mass conservation equations**

$$\partial_t \rho + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}) = 0$$

- **Momentum conservation equation**

$$\partial_t(\rho \boldsymbol{v}) + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}\otimes\boldsymbol{v}) + \boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{P}} = 0 \qquad \boldsymbol{\mathcal{P}} = \boldsymbol{\mathcal{P}}^{\mathrm{K}} + \boldsymbol{\mathcal{P}}^{\mathrm{P}}$$

$$\boldsymbol{\mathcal{P}}^{\mathrm{K}}(\mathbf{r},t) = \int m(\boldsymbol{c}_1 - \boldsymbol{v})\otimes(\boldsymbol{c}_1 - \boldsymbol{v}) f_1(\mathbf{r},\boldsymbol{c}_1,t)\mathrm{d}\boldsymbol{c}_1$$

$$\boldsymbol{\mathcal{P}}^{\mathrm{P}}(\mathbf{r},t) = -\tfrac{1}{2}\int \frac{\varphi'(r_{12})}{r_{12}}\,\mathbf{r}_{12}\otimes\mathbf{r}_{12}\; n_{12}\big(\mathbf{r}-(1-\alpha)\mathbf{r}_{12}, \mathbf{r}+\alpha\mathbf{r}_{12}, t\big)\mathrm{d}\alpha\mathrm{d}\mathbf{r}_{12}$$

Kinetic framework (7)

- **Energy conservation equation**

$$\partial_t \mathcal{E} + \boldsymbol{\nabla}\boldsymbol{\cdot}(\boldsymbol{v}\mathcal{E}) + \boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\mathcal{Q}} = -\boldsymbol{\mathcal{P}}\boldsymbol{:}\boldsymbol{\nabla}\boldsymbol{v} \qquad \boldsymbol{\mathcal{Q}} = \boldsymbol{\mathcal{Q}}^{\mathrm{K}} + \boldsymbol{\mathcal{Q}}_1^{\mathrm{P}} + \boldsymbol{\mathcal{Q}}_2^{\mathrm{P}}$$

$$\boldsymbol{\mathcal{Q}}^{\mathrm{K}}(\mathbf{r},t) = \tfrac{1}{2}\int m|\boldsymbol{c}_1 - \boldsymbol{v}|^2(\boldsymbol{c}_1 - \boldsymbol{v}) f_1(\mathbf{r},\boldsymbol{c}_1,t)\mathrm{d}\boldsymbol{c}_1$$

$$\boldsymbol{\mathcal{Q}}_1^{\mathrm{P}}(\mathbf{r},t) = \tfrac{1}{2}\int \varphi(r_{12})(\boldsymbol{c}_1 - \boldsymbol{v}) f_2(\mathbf{r},\boldsymbol{c}_1,\mathbf{r}+\mathbf{r}_{12},\boldsymbol{c}_2,t)\mathrm{d}\boldsymbol{c}_1\mathrm{d}\mathbf{r}_{12}\mathrm{d}\boldsymbol{c}_2$$

$$\boldsymbol{\mathcal{Q}}_2^{\mathrm{P}}(\mathbf{r},t) = -\tfrac{1}{4}\int \frac{\varphi'(r_{12})}{r_{12}}\mathbf{r}_{12}\,\mathbf{r}_{12}\boldsymbol{\cdot}(\boldsymbol{c}_1 - \boldsymbol{v} + \boldsymbol{c}_2 - \boldsymbol{v})$$

$$\times\; f_2\big(\mathbf{r}-(1-\alpha)\mathbf{r}_{12},\boldsymbol{c}_1,\mathbf{r}+\alpha\mathbf{r}_{12},\boldsymbol{c}_2,t\big)\mathrm{d}\alpha\mathrm{d}\boldsymbol{c}_1\mathrm{d}\mathbf{r}_{12}\mathrm{d}\boldsymbol{c}_2$$

Kinetic framework (8)

- **BBGKY hierarchy and moderately dense gas kinetic theory**

  Yvon (1935), Born and Green (1946), Kirkwood (1946), Bogoliubov (1946)

  Choh and Uhlenbeck (1958) García-Colín et al. (1966) Cohen et al. (1970)

  Chapman and Cowling (1970) Ferziger and Kaper (1972)

- **Kinetic entropy (no known general H theorem)**

$$
\begin{aligned}
\mathcal{S}^{\mathrm{K}}(\mathbf{r},t) = & -k_{\mathrm{B}} \int f_1(\mathbf{r},\boldsymbol{c}_1,t)\Big(\log \frac{h_{\mathrm{P}}^3 f_1(\mathbf{r},\boldsymbol{c}_1,t)}{m^3} - 1\Big)\mathrm{d}\boldsymbol{c}_1 \\
& - \tfrac{1}{2}k_{\mathrm{B}} \int \Big(f_2(\mathbf{r},\boldsymbol{c}_1,\mathbf{r}+\mathbf{r}_{12},\boldsymbol{c}_2,t)\Big(\log \frac{f_2(\mathbf{r},\boldsymbol{c}_1,\mathbf{r}+\mathbf{r}_{12},\boldsymbol{c}_2,t)}{f_1(\mathbf{r},\boldsymbol{c}_1,t)f_1(\mathbf{r}+\mathbf{r}_{12},\boldsymbol{c}_2,t)} - 1\Big) \\
& + f_1(\mathbf{r},\boldsymbol{c}_1,t)f_1(\mathbf{r}+\mathbf{r}_{12},\boldsymbol{c}_2,t)\Big)\mathrm{d}\boldsymbol{c}_1\mathrm{d}\mathbf{r}_{12}\mathrm{d}\boldsymbol{c}_2
\end{aligned}
$$

  Stratonovich (1955) Nettleton and Green (1958) Klimontovitch (1972)

Classical Nonideal Fluids (0)

- **New Enskog scaling**

$$\partial_t f_1 + \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} f_1 = \frac{1}{\epsilon} \mathcal{J}^{(0)}(f) + \mathcal{J}^{(1)}(f)$$

$$f_1 = f_1^{(0)}\big(1 + \epsilon \phi^{(1)} + \mathcal{O}(\epsilon^2)\big)$$

- **Zeroth order distributions**

$$\mathcal{J}^{(0)}\big(f^{(0)}\big) = 0$$

$$f_1^{(0)} = n\Big(\frac{m}{2\pi k_{\mathrm{B}} T}\Big)^{\frac{3}{2}} \exp\Big(-\frac{m|\boldsymbol{c}_1 - \boldsymbol{v}|^2}{2k_{\mathrm{B}} T}\Big)$$

- **Various choices for zeroth order and pair distribution functions $\boldsymbol{f_2^{(0)}}$**

Classical Nonideal Fluids (1)

- **Classic zeroth order pair distributions**

$$f_2^{(0),\mathrm{cl}} = f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_1', t)\, f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_2', t) = f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_1, t) f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_2, t)\mathfrak{g}(\mathbf{r}_1, r_{12})$$

$$\mathfrak{g}(\mathbf{r}_1, r_{12}) = \exp\Big(-\frac{\varphi(r_{12})}{k_{\mathrm{B}} T(\mathbf{r}_1)}\Big)$$

$$m\boldsymbol{c}_1 + m\boldsymbol{c}_2 = m\boldsymbol{c}_1' + m\boldsymbol{c}_2'$$

$$\tfrac{1}{2}m|\boldsymbol{c}_1|^2 + \tfrac{1}{2}m|\boldsymbol{c}_2|^2 + \varphi(r_{12}) = \tfrac{1}{2}m|\boldsymbol{c}_1'|^2 + \tfrac{1}{2}m|\boldsymbol{c}_2'|^2$$

- **Euler equations**

$$\partial_t \rho + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}) = 0$$

$$\partial_t(\rho \boldsymbol{v}) + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}\otimes\boldsymbol{v}) + \boldsymbol{\nabla} p^{\mathrm{cl}} = 0$$

$$\partial_t \mathcal{E}^{\mathrm{cl}} + \boldsymbol{\nabla}\cdot\big(\boldsymbol{v}\mathcal{E}^{\mathrm{cl}}\big) + p^{\mathrm{cl}}\boldsymbol{\nabla}\cdot\boldsymbol{v} = 0$$

Classical Nonideal Fluids (2)

- **Mayer function moments**

$$\mathfrak{f}_{12}(\mathbf{r}_1, r_{12}) = \exp\Big(-\frac{\varphi(r_{12})}{k_B T(\mathbf{r}_1)}\Big) - 1 \qquad \beta = \int \mathfrak{f}_{12} \mathrm{d}\mathbf{r}_{12} \qquad \beta' = \mathrm{d}\beta/\mathrm{d}(k_B T)$$

- **Thermodynamic properties**

$$p^{\mathrm{cl}} = n k_B T - \tfrac{1}{2} n^2 \beta\, k_B T$$

$$\mathcal{E}^{\mathrm{cl}} = \tfrac{3}{2} n k_B T + \tfrac{1}{2} n^2 \beta' (k_B T)^2$$

$$\mathcal{S}^{\mathrm{cl}} = -k_B n \Big(\log(n\Lambda^3) - \tfrac{5}{2}\Big) + \tfrac{1}{2} k_B n^2 (\beta + k_B T \beta')$$

Λ De Broglie thermal wavelength $\Lambda = h_P/(2\pi m k_B T)^{1/2}$

Classical Nonideal Fluids (3)

- **Linearized equations**

$$\mathcal{I}(\phi^{(1)}) = \psi_i^{(1)}$$

$$\psi^{(1)} = -\Big(\partial_t \log f_1^{(0)} + \boldsymbol{c}_1 \cdot \boldsymbol{\nabla}_{\mathbf{r}_1} \log f_1^{(0)}\Big) + \frac{1}{f_1^{(0)}} \mathcal{J}^{(1)}(f_1^{(0)})$$

- **Evaluation of linearized equations**

  $\mathcal{I}$ coincide with Boltzmann linearized operator

  First order Taylor expansions of pair distributions

$$\psi^{(1)} = -\psi^{\eta} \boldsymbol{:} \boldsymbol{\nabla} \boldsymbol{v} - \psi^{\kappa} \boldsymbol{\nabla} \cdot \boldsymbol{v} - \psi^{\lambda} \cdot \boldsymbol{\nabla} \Big(\frac{-1}{k_{\mathrm{B}} T}\Big)$$

  New nonlocal collision integrals

  Simplified Enskog constraints

Classical Nonideal Fluids (4)

- **Decomposition the perturbed distribution**

$$\phi = -\phi^{\eta}\boldsymbol{:}\boldsymbol{\nabla}\boldsymbol{v} - \phi^{\kappa}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{v} - \phi^{\lambda}\boldsymbol{\cdot}\boldsymbol{\nabla}\Big(\frac{-1}{k_{\rm B}T}\Big)$$

- **First order equations**

$$\partial_t\rho + \boldsymbol{\nabla}\boldsymbol{\cdot}(\rho\boldsymbol{v}) = 0$$

$$\partial_t(\rho\boldsymbol{v}) + \boldsymbol{\nabla}\boldsymbol{\cdot}(\rho\boldsymbol{v}\otimes\boldsymbol{v}) + \boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\mathcal{P}} = 0$$

$$\partial_t\mathcal{E} + \boldsymbol{\nabla}\boldsymbol{\cdot}(\boldsymbol{v}\mathcal{E}) + \boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\mathcal{Q}} = -\boldsymbol{\mathcal{P}}\boldsymbol{:}\boldsymbol{\nabla}\boldsymbol{v}$$

- **Transport fluxes**

$$\boldsymbol{\mathcal{P}} = p^{\rm cl}\boldsymbol{I} - \mathfrak{v}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{v}\,\boldsymbol{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^{t} - \tfrac{2}{3}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{v}\,\boldsymbol{I}\big)$$

$$\boldsymbol{\mathcal{Q}} = -\lambda\boldsymbol{\nabla}T$$

Very complex expressions for the transport coefficients

Classical Nonideal Fluids (5)

- **Van der Waals equation of state**

$$\varphi(r_{12}) = \begin{cases} +\infty & \text{if } 0 \le r_{12} \le \sigma \\ \varphi(r_{12}) < \infty & \text{if } \sigma < r_{12} \end{cases} \qquad \beta = \int \mathfrak{f}_{12} \mathrm{d}\mathbf{r}_{12}$$

$$p^{\mathrm{cl}} = \frac{n k_{\mathrm{B}} T}{1 - \mathsf{b} n} - n^2 \mathsf{a}$$

$$\mathsf{b} = 4 \frac{4\pi\sigma^3}{3} \qquad \mathsf{a} = -2\pi \int_{2\sigma}^{\infty} \varphi(r_{12}) r_{12}^2 \mathrm{d}r_{12}$$

- **Orders of magnitude**

$$\sigma^\star \ll r^\star \ll l_{\mathrm{K}}^\star \qquad \sigma^{\star 2} l_{\mathrm{K}}^\star = r^{\star 3} \qquad \beta^\star = \sigma^{\star 3}$$

$$\tfrac{1}{2} n^2 \beta k_{\mathrm{B}} T \Big/ n k_{\mathrm{B}} T \approx \left(\frac{\sigma^\star}{r^\star} \right)^3$$

Kinetic Derivation for Diffuse Interface Fluids (1)

- **Higher order Taylor expansions of symmetrized pair distributions**

$$f_2^{(0),\mathrm{cl}} = f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_1, t) f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_2, t)\mathfrak{g}(\mathbf{r}_1, r_{12}) \qquad \mathfrak{g}(\mathbf{r}_1, r_{12}) = \exp\Big(-\frac{\varphi(r_{12})}{k_{\mathrm{B}} T(\mathbf{r}_1)}\Big)$$

$$f_2^{(0),\mathrm{sy}} = f_1^{(0)}(\mathbf{r}_1, \boldsymbol{c}_1, t) f_1^{(0)}(\mathbf{r}_2, \boldsymbol{c}_2, t)\mathfrak{g}(\overline{\mathbf{r}}_{i,j}, r_{12}) \qquad \mathfrak{g} = \mathfrak{g}(r_{12}) = \mathfrak{g}(\mathbf{r}_1, r_{12})$$

- **Potential part of the pressure tensor**

$$\boldsymbol{\mathcal{P}}^{\mathrm{P}}(\mathbf{r}, t) = -\tfrac{1}{2} \int \frac{\varphi'(r_{12})}{r_{12}}\, \mathbf{r}_{12}\otimes\mathbf{r}_{12}\; n_{12}\big(\mathbf{r} - (1-\alpha)\mathbf{r}_{12}, \mathbf{r} + \alpha\mathbf{r}_{12}, t\big)\mathrm{d}\alpha\mathrm{d}\mathbf{r}_{12}$$

$$n_{12}\big(\mathbf{r}_1 - (1-\alpha)\mathbf{r}_{12}, \mathbf{r}_1 + \alpha\mathbf{r}_{12}, t\big) \approx$$

$$\big(n(\mathbf{r}_1) - (1-\alpha)\boldsymbol{\nabla} n(\mathbf{r}_1)\cdot\mathbf{r}_{12} + \tfrac{1}{2}(1-\alpha)^2\boldsymbol{\nabla}^2 n(\mathbf{r}_1):(\mathbf{r}_{12}\otimes\mathbf{r}_{12})\big)$$

$$\times\; \big(n(\mathbf{r}_1) + \alpha\boldsymbol{\nabla} n(\mathbf{r}_1)\cdot\mathbf{r}_{12} + \tfrac{1}{2}\alpha^2\boldsymbol{\nabla}^2 n(\mathbf{r}_1):(\mathbf{r}_{12}\otimes\mathbf{r}_{12})\big) \times \mathfrak{g}(r_{12})$$

Kinetic Derivation for Diffuse Interface Fluids (2)

- **Extra terms with two derivative $\boldsymbol{\mathcal{P}}^{\rm ex}$ in the pressure tensor $\boldsymbol{\mathcal{P}}$**

  Lengthy calculations of all contributions

  $$\boldsymbol{\mathcal{P}}^{\rm ex} = \tfrac{\overline{\varkappa}}{6}\Big(2\boldsymbol{\nabla} n \otimes \boldsymbol{\nabla} n + \boldsymbol{\nabla} n \cdot \boldsymbol{\nabla} n \boldsymbol{I} - 4n\boldsymbol{\nabla}^2 n - 2n\Delta n \boldsymbol{I}\Big)$$

  $$\overline{\varkappa} = \frac{1}{30}\int \varphi'(r_{12})\mathfrak{g}(r_{12}) r_{12}^3 {\rm d}\mathbf{r}_{12} = \frac{2\pi}{15}\int \varphi'(r_{12})\mathfrak{g}(r_{12}) r_{12}^5 {\rm d}r_{12}$$

  Integro-differential relations and equivalent formulation $\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{P}}^{\rm ex} = \boldsymbol{\nabla}\cdot\overline{\boldsymbol{\mathcal{P}}}^{\rm ex}$

  Neglect temperature dependence of the capillarity coefficients $\overline{\varkappa} = \varkappa/m^2$

- **The Korteweg tensor**

  $$\overline{\boldsymbol{\mathcal{P}}}^{\rm ex} = \overline{\varkappa}\Big(\boldsymbol{\nabla} n \otimes \boldsymbol{\nabla} n - \tfrac{1}{2}|\boldsymbol{\nabla} n|^2 \boldsymbol{I} - n\Delta n \boldsymbol{I}\Big) = \varkappa\Big(\boldsymbol{\nabla}\rho \otimes \boldsymbol{\nabla}\rho - \tfrac{1}{2}|\boldsymbol{\nabla}\rho|^2 \boldsymbol{I} - n\Delta n \boldsymbol{I}\Big)$$

Kinetic Derivation for Diffuse Interface Fluids (3)

- **Alternative expressions for the capillarity**

$$\overline{\varkappa} = \tfrac{1}{6} k_{\rm B} T \int \mathfrak{f}_{12} r_{12}^2 \mathrm{d}\mathbf{r}_{12} = \tfrac{2\pi}{3} k_{\rm B} T \int \mathfrak{f}_{12} r_{12}^4 \mathrm{d} r_{12}$$

The potential is such that $\varphi(r_{12}) = \begin{cases} +\infty & \text{if } 0 \leq r_{12} \leq \sigma \\ \varphi(r_{12}) < \infty & \text{if } \sigma < r_{12} \end{cases}$

Linearizing $\mathfrak{f}_{12}$ over $r_{12} > \sigma$ yields $\overline{\varkappa} = -\frac{1}{6} \int_{r_{12} > \sigma} \varphi r_{12}^2 \mathrm{d}\mathbf{r}_{12}$

- **Orders of magnitude**

$\overline{\varkappa}^\star = k_{\rm B} T^\star \sigma^{\star 5}$ $\qquad$ $\beta^\star = \sigma^{\star 3}$ $\qquad$ $l^\star_{\nabla n}$ Typical length of density gradients

$$\overline{\varkappa} \, |\boldsymbol{\nabla} n|^2 \Big/ n k_{\rm B} T \approx \left(\frac{\sigma^\star}{r^\star} \right)^3 \left(\frac{\sigma^\star}{l^\star_{\nabla n}} \right)^2$$

Kinetic Derivation for Diffuse Interface Fluids (4)

- **Extra terms with two derivatives $\mathcal{E}^{\rm ex}$ in the internal energy $\mathcal{E}$**

$$\mathcal{E}^{\rm ex} = -\tfrac{1}{2}\overline{\varkappa}\, n\Delta n = \tfrac{1}{2}\overline{\varkappa}\,|\boldsymbol{\nabla} n|^2 - \tfrac{1}{2}\boldsymbol{\nabla\cdot}\big(\overline{\varkappa} n \boldsymbol{\nabla} n\big)$$

- **Van der Waals gradient internal energy $\overline{\mathcal{E}}^{\rm ex}$**

$$\overline{\mathcal{E}}^{\rm ex} = \tfrac{1}{2}\overline{\varkappa}\,|\boldsymbol{\nabla} n|^2 = \tfrac{1}{2}\varkappa\,|\boldsymbol{\nabla}\rho|^2 \qquad\qquad \mathcal{E} = \mathcal{E}^{\rm cl} + \overline{\mathcal{E}}^{\rm ex}$$

$$\Xi = -\tfrac{1}{2}\Big(\partial_t \boldsymbol{\nabla\cdot}(\overline{\varkappa} n \boldsymbol{\nabla} n) + \boldsymbol{\nabla\cdot}\big(\boldsymbol{\nabla\cdot}(\overline{\varkappa} n \boldsymbol{\nabla} n)\boldsymbol{v}\big)\Big) = \boldsymbol{\nabla\cdot}\mathfrak{q}_0$$

Kinetic Derivation for Diffuse Interface Fluids (5)

- **Extra terms with two derivatives $\boldsymbol{\mathcal{Q}}^{\rm ex}$ in the heat flux $\boldsymbol{\mathcal{Q}}$**

  Very lengthy calculations all contributions

$$
\begin{aligned}
\boldsymbol{\mathcal{Q}}^{\rm ex} + \boldsymbol{\mathcal{P}}^{\rm ex}\cdot\boldsymbol{v} &= \overline{\varkappa}\, n \boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla} n + \tfrac{1}{2}\overline{\varkappa}\, n^2 \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}) + \tfrac{1}{2}\overline{\varkappa}\, n (\boldsymbol{\nabla}\boldsymbol{v})^t\cdot\boldsymbol{\nabla} n \\
&+ \tfrac{1}{2}\overline{\varkappa}\Big(\boldsymbol{\nabla} n_i \otimes \boldsymbol{\nabla} n + n\boldsymbol{\nabla}^2 n - \boldsymbol{\nabla} n\cdot\boldsymbol{\nabla} n \boldsymbol{I} - n\Delta n\Big)\cdot\boldsymbol{v} \\
&- \frac{\overline{\varkappa}}{6} n \Big(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t + \boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{I}\Big)\cdot\boldsymbol{\nabla} n - \frac{\overline{\varkappa}}{6} n^2 \Big(\Delta\boldsymbol{v} + 2\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v})\Big) \\
&+ \frac{\overline{\varkappa}}{6}\Big(2\boldsymbol{\nabla} n \otimes \boldsymbol{\nabla} n + \boldsymbol{\nabla} n\cdot\boldsymbol{\nabla} n \boldsymbol{I} - 4n\boldsymbol{\nabla}^2 n - 2n\Delta n \boldsymbol{I}\Big)\cdot\boldsymbol{v}
\end{aligned}
$$

Kinetic Derivation for Diffuse Interface Fluids (6)

- **Equivalent formulation with $\boldsymbol{\nabla}\cdot(\boldsymbol{\mathcal{Q}}^{\mathbf{ex}} + \boldsymbol{\mathcal{P}}^{\mathbf{ex}}\cdot\boldsymbol{v}) = \boldsymbol{\nabla}\cdot(\overline{\boldsymbol{\mathcal{Q}}}^{\mathbf{ex}} + \overline{\boldsymbol{\mathcal{P}}}^{\mathbf{ex}}\cdot\boldsymbol{v})$**

$$\begin{aligned}\boldsymbol{\nabla}\cdot(\boldsymbol{\mathcal{Q}}^{\mathrm{ex}} + \boldsymbol{\mathcal{P}}^{\mathrm{ex}}\cdot\boldsymbol{v}) = \boldsymbol{\nabla}\cdot\Big(&\overline{\varkappa}\, n\boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla} n - \tfrac{1}{3}\overline{\varkappa}\, n\boldsymbol{\nabla}\boldsymbol{v}\cdot\boldsymbol{\nabla} n \\ &+ \tfrac{1}{3}\overline{\varkappa}\, n(\boldsymbol{\nabla}\boldsymbol{v})^t\cdot\boldsymbol{\nabla} n - \tfrac{1}{6}\overline{\varkappa} n^2\Delta\boldsymbol{v} + \tfrac{1}{6}\overline{\varkappa}\, n^2\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}) \\ &+ \overline{\varkappa}\,\big(\boldsymbol{\nabla} n\otimes\boldsymbol{\nabla} n - \tfrac{1}{2}\boldsymbol{\nabla} n\cdot\boldsymbol{\nabla} n\boldsymbol{I} - n\Delta n\boldsymbol{I}\big)\cdot\boldsymbol{v}\Big)\end{aligned}$$

- **The Dunn and Serrin heat flux**

$$\overline{\boldsymbol{\mathcal{Q}}}^{\mathrm{ex}} = \overline{\varkappa} n\boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla} n = \varkappa\rho\boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla}\rho$$

- **Zeroth order resulting equations**

  Euler equation

  Van der Waals/Cahn-Hilliard internal energy

  Korteweg tensor and Dunn and Serrin heat flux

Kinetic Derivation for Diffuse Interface Fluids (7)

- **First order equations**

$$\partial_t \rho + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}) = 0,$$

$$\partial_t(\rho \boldsymbol{v}) + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}\otimes\boldsymbol{v}) + \boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{P}} = 0$$

$$\partial_t \mathcal{E} + \boldsymbol{\nabla}\cdot(\boldsymbol{v}\mathcal{E}) + \boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{Q}} = -\boldsymbol{\mathcal{P}}:\boldsymbol{\nabla}\boldsymbol{v}$$

- **Transport fluxes at first order**

$$\begin{aligned}\boldsymbol{\mathcal{P}} =& p^{\mathrm{cl}}\boldsymbol{I} - \mathfrak{v}\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\boldsymbol{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^t - \tfrac{2}{3}\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\boldsymbol{I}\big)\\ &+ \varkappa\Big(\boldsymbol{\nabla}\rho\otimes\boldsymbol{\nabla}\rho - \tfrac{1}{2}|\boldsymbol{\nabla}\rho|^2\boldsymbol{I} - \rho\Delta\rho\boldsymbol{I}\Big)\end{aligned}$$

$$\boldsymbol{\mathcal{Q}} = -\lambda\boldsymbol{\nabla}T + \varkappa\rho\boldsymbol{\nabla}\cdot\boldsymbol{v}\boldsymbol{\nabla}\rho$$

Compatibility with Thermodynamics (1)

- **Gibbs relation from $\boldsymbol{\mathcal{A} = \mathcal{A}^{\text{cl}} + \frac{1}{2}\varkappa|\nabla\rho|^2}$**

$$T\mathrm{d}\mathcal{S} = \mathrm{d}\mathcal{E} - g\mathrm{d}\rho - \varkappa\boldsymbol{\nabla}\rho\boldsymbol{\cdot}\mathrm{d}\boldsymbol{\nabla}\rho$$

- **Entropy production**

$$\partial_t\mathcal{S} + \boldsymbol{\nabla\cdot}(\boldsymbol{v}\mathcal{S}) + \boldsymbol{\nabla\cdot}\Big(\frac{\boldsymbol{\mathcal{Q}}}{T} - \frac{\varkappa\rho\boldsymbol{\nabla\cdot v}\boldsymbol{\nabla}\rho}{T}\Big)$$
$$= -\frac{1}{T}\Big(\boldsymbol{\mathcal{P}} - p\boldsymbol{I} - \varkappa\boldsymbol{\nabla}\rho\otimes\boldsymbol{\nabla}\rho + \rho\boldsymbol{\nabla\cdot}(\varkappa\boldsymbol{\nabla}\rho)\,\boldsymbol{I}\Big)\boldsymbol{:}\boldsymbol{\nabla v} - \Big(\boldsymbol{\mathcal{Q}} - \varkappa\rho\boldsymbol{\nabla\cdot v}\boldsymbol{\nabla}\rho\Big)\boldsymbol{\cdot\nabla}\Big(\frac{-1}{T}\Big)$$

- **Ambiguity of thermodynamical methods**

$$\varkappa\rho\boldsymbol{\nabla\cdot v}\boldsymbol{\nabla}\rho\boldsymbol{\cdot\nabla}\Big(\frac{-1}{T}\Big)$$

Compatibility with Thermodynamics (2)

- **Thermodynamic of irreversible processes**

  Equations compatible with the thermodynamic of irreversible processes

  Thermodynamic of irreversible processes *ambiguous* for diffuse interface fluids

  Gibbsian entropy $\mathcal{S}$ differ from $\int \mathcal{S}^{\mathrm{K}} \mathrm{d}\boldsymbol{c}_1$ with capillarity effects

- **Agreement with Bogoliubov pair distributions**

  Bogoliubov zeroth order pair distributions $f_2^{(0),\mathrm{Bo}} = f_1^{(0)}(\mathbf{r}_1', \boldsymbol{c}_1') f_1^{(0)}(\mathbf{r}_2', \boldsymbol{c}_2')$

  $l^\star_{\nabla T}$ and $l^\star_{\nabla T}$ characteristic lengths of temperature and velocity gradients

$$\Big(\frac{\sigma^\star}{r^\star}\Big)^3 \Big(\frac{\sigma^\star}{l^\star_{\nabla n}}\Big) \Big(\frac{\sigma^\star}{l^\star_{\nabla T}}\Big) \ll 1 \qquad \Big(\frac{\sigma^\star}{r^\star}\Big)^3 \Big(\frac{\sigma^\star}{l^\star_{\nabla n}}\Big) \Big(\frac{\sigma^\star}{l^\star_{\nabla v}}\Big) \Big(\frac{\delta v^\star}{\sqrt{k_{\mathrm{B}} T^\star / m^\star}}\Big) \ll 1$$

  $f_1^{(0)} = n \widetilde{f}_1^{(0)}$ $\qquad \boldsymbol{\nabla} \log \widetilde{f}_1^{(0)} \ll \boldsymbol{\nabla} \log n$ $\qquad$ Hard potential approximations

  Careful estimates for deviations in $\mathcal{E}$, $\boldsymbol{\mathcal{P}}$, $\boldsymbol{\mathcal{Q}}_1^{\mathrm{P}}$, $\boldsymbol{\mathcal{Q}}_2^{\mathrm{P}}$, and $\psi^{(1)}$

Agreement with Bogoliubov Distribution

- **Rescaled distributions**

$$T(\mathbf{r}_1) = T(\mathbf{r}_1') = T(\mathbf{r}_2) = T(\mathbf{r}_2') = \overline{T} \qquad f_1^{(0)} = n_i\, \widetilde{f}_i^{(0)}$$

$$\boldsymbol{v}(\mathbf{r}_1) = \overline{\boldsymbol{v}} + \delta\boldsymbol{v}_1 \quad \boldsymbol{v}(\mathbf{r}_1') = \overline{\boldsymbol{v}} + \delta\boldsymbol{v}_1' \quad \boldsymbol{v}(\mathbf{r}_2) = \overline{\boldsymbol{v}} + \delta\boldsymbol{v}_2 \quad \boldsymbol{v}(\mathbf{r}_2') = \overline{\boldsymbol{v}} + \delta\boldsymbol{v}_2'$$

All relative Mach numbers negligible $\delta\boldsymbol{v}_i\sqrt{m/2k_{\mathrm{B}}T(\mathbf{r})} \ll 1$

$$\widetilde{f}_i^{(0)}(\mathbf{r}_1',\boldsymbol{c}_1')\widetilde{f}_i^{(0)}(\mathbf{r}_2',\boldsymbol{c}_2') = \mathfrak{g}\Big(\frac{m}{2\pi k_{\mathrm{B}}\overline{T}}\Big)^3 \exp\Big(-\frac{m|\boldsymbol{c}_1-\overline{\boldsymbol{v}}|^2 + m|\boldsymbol{c}_2-\overline{\boldsymbol{v}}|^2}{2k_{\mathrm{B}}\overline{T}}\Big)$$

$$\widetilde{f}_i^{(0)}(\mathbf{r}_1',\boldsymbol{c}_1')\widetilde{f}_i^{(0)}(\mathbf{r}_2',\boldsymbol{c}_2') = \mathfrak{g}\widetilde{f}_i^{(0)}(\mathbf{r}_1,\boldsymbol{c}_1)\widetilde{f}_i^{(0)}(\mathbf{r}_2,\boldsymbol{c}_2)$$

- **Hard potential approximation for number densities**

$$n(\mathbf{r}_1')n(\mathbf{r}_2') = n(\mathbf{r}_1)n(\mathbf{r}_2)$$

$$f_2^{(0),\mathrm{Bo}} = \mathfrak{g} f_1^{(0)}(\mathbf{r}_1,\boldsymbol{c}_1) f_1^{(0)}(\mathbf{r}_2,\boldsymbol{c}_2) = f_2^{(0),\mathrm{sy}}$$

4 Augmented System

Augmented Systems for Diffuse Interface Models

- **Augmented systems**

  Gavrilyuk and Gouin (1999) Benzoni et al. (2005) (2006) (2007)
  Bresch et al. (2019) (2000) Kotschote (2012)

- **Two velocity hydrodynamics**

  Bresch et al. (2008) (2015) (2015)

- **Symmetrization of the augmented system**

  Gavrilyuk and Gouin (1999) (2000)

Augmented system (1)

- **Extra unknown** $\boldsymbol{w} = \boldsymbol{\nabla}\rho$

$$\partial_t \boldsymbol{w} + \sum_{i\in\mathcal{D}} \partial_i\big(\boldsymbol{w}\, v_i + \rho\boldsymbol{\nabla} v_i\big) = 0 \qquad \mathcal{D} = \{\,1,\ldots,d\,\}$$

- **Augmented unknowns**

$$\mathsf{u} = \big(\rho, \boldsymbol{w}, \rho\boldsymbol{v}, \mathcal{E} + \tfrac{1}{2}\rho|\boldsymbol{v}|^2\big)^t \qquad \mathsf{z} = \big(\rho, \boldsymbol{w}, \boldsymbol{v}, T\big)^t$$

- **New thermodynamic functions**

$$\mathcal{E} = \mathcal{E}^{\mathrm{cl}} + \tfrac{1}{2}(\varkappa - T\partial_T\varkappa)|\boldsymbol{w}|^2 \qquad \mathcal{S} = \mathcal{S}^{\mathrm{cl}} - \tfrac{1}{2}\partial_T\varkappa|\boldsymbol{w}|^2$$

$$p = p^{\mathrm{cl}} - \tfrac{1}{2}\varkappa|\boldsymbol{w}|^2 \qquad g = g^{\mathrm{cl}} \qquad \mathcal{H} = \mathcal{H}^{\mathrm{cl}} - \tfrac{1}{2}T\partial_T\varkappa|\boldsymbol{w}|^2$$

Augmented system (2)

- **Thermodynamic functions**

(H₁) *$\mathcal{E}$, p, $\mathcal{S}$ are C^γ functions of* $\mathsf{z} \in \mathcal{O}_{\mathsf{z}} \subset (0,\infty) \times \mathbb{R}^d \times \mathbb{R}^d \times (0,\infty)$ *open set*

$\varkappa = \varkappa(T)$ *is a $C^{\gamma+1}$ function of temperature T over $\mathcal{O}_{\mathsf{z}}$*

If $(\rho, T)^t \in \mathcal{O}_{\mathsf{z}^{\mathrm{cl}}}$, $(\rho, 0, 0, T)^t \in \mathcal{O}_{\mathsf{z}}$. *If* $(\rho, \boldsymbol{w}, \boldsymbol{v}, T)^t \in \mathcal{O}_{\mathsf{z}}$, $(\rho, T)^t \in \mathcal{O}_{\mathsf{z}^{\mathrm{cl}}}$

(H_2) *Letting* $\mathcal{G} = \mathcal{E} + p - T\mathcal{S} = \rho g$ *we have* $T\, d\mathcal{S} = d\mathcal{E} - g\, d\rho - \varkappa \boldsymbol{w} \cdot d\boldsymbol{w}$

(H_3) *The open set $\mathcal{O}_{\mathsf{z}}$ is increasing with temperature T and* $\partial_T \mathcal{E} > 0$

(H_4) *The capillarity coefficient is positive* $\varkappa > 0$ *over* $\mathcal{O}_{\mathsf{z}}$

(H_5) *The coefficients* $\mathfrak{v}$, η *and* λ *are* C^γ *functions over* $\mathcal{O}_{\mathsf{z}}$

We have $\eta > 0$, $\lambda > 0$, $\mathfrak{v} \geq 0$, *and* $\mathfrak{v} + \eta(1 - \frac{2}{d}) > 0$

Augmented system (3)

Lemma 1. *Assuming* (H_1)-(H_2) *and that* $\mathsf{z} \mapsto \mathsf{u}$ *is locally invertible then*

$$\partial^2_{\mathsf{uu}}\mathcal{S} \text{ negative definite} \iff \partial_T \mathcal{E} > 0 \quad \partial_\rho p > 0 \quad \text{and} \quad \varkappa > 0$$

Lemma 2. *Assuming* (H_1)-(H_3) *then the map* $\mathsf{z} \mapsto \mathsf{u}$ *is a* C^γ *diffeomorphism from the open set* $\mathcal{O}_\mathsf{z}$ *onto an open set* $\mathcal{O}_\mathsf{u}$.

Lemma 3. *Assuming* (H_1) *and given* $\delta > 0$ *there exists a* $C^{\gamma-1}$ *function* m *such that* $\mathsf{m} \geq 0$

$$\mathsf{m} + \partial_\rho p/\rho T > 0$$

and $\mathsf{m} = 0$ *if* $\partial_\rho p/\rho T \geq \delta$.

Augmented system (4)

- **Partial differential equations**

$$\partial_t \rho + \sum_{i \in \mathcal{D}} \partial_i (\rho v_i) = 0$$

$$\partial_t w_j + \sum_{i \in \mathcal{D}} \partial_i \big(w_j \, v_i + \rho \partial_j v_i \big) = 0$$

$$\partial_t (\rho v_j) + \sum_{i \in \mathcal{D}} \partial_i (\rho v_i v_j + \mathcal{P}_{ij}) = 0$$

$$\partial_t \big(\mathcal{E} + \tfrac{1}{2} \rho |\boldsymbol{v}|^2 \big) + \sum_{i \in \mathcal{D}} \partial_i \Big((\mathcal{E} + \tfrac{1}{2} \rho |\boldsymbol{v}|^2) v_i + \mathcal{Q}_i + \sum_{i \in \mathcal{D}} \mathcal{P}_{ij} v_j \Big) = 0$$

Augmented system (5)

- **Transport fluxes**

$$\mathcal{P}_{ij} = p\delta_{ij} + \varkappa\partial_i\rho\,\partial_j\rho - \rho\sum_{l\in\mathcal{D}}\partial_l(\varkappa\partial_l\rho)\delta_{ij} + \mathcal{P}_{ij}^{\rm d}$$

$$\mathcal{Q}_i = \varkappa\rho\sum_{l\in\mathcal{D}}\partial_l v_l\,\partial_i\rho + \mathcal{Q}_i^{\rm d}$$

- **Dissipative transport fluxes**

$$\mathcal{P}_{ij}^{\rm d} = -\,\mathfrak{v}\sum_{l\in\mathcal{D}}\partial_l v_l\,\delta_{ij} - \eta\big(\partial_i v_j + \partial_j v_i - \tfrac{2}{d}\sum_{l\in\mathcal{D}}\partial_l v_l\,\delta_{ij}\big) \qquad \mathcal{Q}_i^{\rm d} = -\lambda\partial_i T$$

Augmented system (6)

- **Augmented entropic variable**

$$\sigma = -\mathcal{S} = -\mathcal{S}^{\mathrm{cl}} + \tfrac{1}{2}\partial_T \varkappa\, |\boldsymbol{w}|^2 \qquad \mathsf{v} = (\partial_{\mathsf{u}}\sigma)^t = \frac{1}{T}\Big(g - \tfrac{1}{2}|\boldsymbol{v}|^2, \varkappa\, \boldsymbol{w}, \boldsymbol{v}, -1\Big)^t$$

- **Stable points**

$$\mathcal{O}_{\mathsf{z}}^{\mathrm{st}} = \{\, \mathsf{z} \in \mathcal{O}_{\mathsf{z}} \;\big|\; \partial_\rho p > 0 \,\}$$

$\mathsf{u} \mapsto \mathsf{v}$ locally invertible around stable points with $\partial_\rho p > 0$

- **Legendre transform $\mathcal{L}$ of entropy**

$$\mathcal{L} = \langle \mathsf{u}, \mathsf{v} \rangle - \sigma = \frac{1}{T}\big(p + \varkappa|\boldsymbol{w}|^2\big) \qquad \partial_{\mathsf{u}}\sigma = \mathsf{v}^t \qquad \partial_{\mathsf{v}}\mathcal{L} = \mathsf{u}^t$$

- **Convective fluxes**

$$\mathsf{F}_i = \Big(\partial_{\mathsf{v}}(\mathcal{L} v_i)\Big)^t \qquad \mathcal{L}_i = \mathcal{L} v_i$$

Augmented system (7)

- **New augmented form**

$$\partial_t \mathsf{u} + \sum_{i\in\mathcal{D}} \partial_i \big(\mathsf{F}_i + \mathsf{F}_i^{\mathrm{d}} + \mathsf{F}_i^{\mathrm{c}}\big) = 0$$

- **New augmented fluxes inthe ith direction**

$$\mathsf{F}_i = \Big(\rho v_i, \boldsymbol{w} v_i, \rho \boldsymbol{v} v_i + (p + \varkappa |\boldsymbol{w}|^2)\mathfrak{b}_i, (\mathcal{E} + p + \varkappa |\boldsymbol{w}|^2) v_i\Big)^t$$

$$\mathsf{F}_i^{\mathrm{d}} = \Big(0, 0_{d,1},\ \boldsymbol{\mathcal{P}}_i^{\mathrm{d}},\ \mathcal{Q}_i^{\mathrm{d}} + \sum_{j\in\mathcal{D}} \mathcal{P}_{ij}^{\mathrm{d}} v_j\Big)^t \qquad \boldsymbol{\mathcal{P}}_i^{\mathrm{d}} = (\mathcal{P}_{1i}^{\mathrm{d}}, \dots, \mathcal{P}_{di}^{\mathrm{d}})^t$$

$$\mathsf{F}_i^{\mathrm{c}} = \Big(0, \rho \boldsymbol{\nabla} v_i, -\rho \boldsymbol{\nabla}(\varkappa w_i), \rho\varkappa \boldsymbol{w}\boldsymbol{\cdot}\boldsymbol{\nabla} v_i - \rho \boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{\nabla}(\varkappa w_i)\Big)^t$$

- **Equivalence of both formulations**

  Rely on calculus identities

Augmented system (8)

- **Convective, dissipative and capillary matrices**

$$\mathsf{A}_i = \partial_{\mathsf{u}} \mathsf{F}_i \qquad \mathsf{F}_i^{\mathrm{d}} = -\sum_{j\in\mathcal{D}} \mathsf{B}_{ij}^{\mathrm{d}} \partial_j \mathsf{u} \qquad \mathsf{F}_i^{\mathrm{c}} = -\sum_{j\in\mathcal{D}} \mathsf{B}_{ij}^{\mathrm{c}} \partial_j \mathsf{u}, \qquad i \in \mathcal{D}$$

- **Quasilinear form**

$$\partial_t \mathsf{u} + \sum_{i\in\mathcal{D}} \mathsf{A}_i(\mathsf{u}) \partial_i \mathsf{u} - \sum_{i,j\in\mathcal{D}} \partial_i \big(\mathsf{B}_{ij}^{\mathrm{d}}(\mathsf{u}) \partial_j \mathsf{u}\big) - \sum_{i,j\in\mathcal{D}} \partial_i \big(\mathsf{B}_{ij}^{\mathrm{c}}(\mathsf{u}) \partial_j \mathsf{u}\big) = 0$$

A_i, $\mathsf{B}_{ij}^{\mathrm{d}}$, and $\mathsf{B}_{ij}^{\mathrm{c}}$, for $i, j \in \mathcal{D}$, have at least regularity $C^{\gamma-1}$ over $\mathcal{O}_{\mathsf{u}}$

- **Symmetrization**

Structure of the system of equations plus existence results

Symmetrized Augmented System (1)

- **Entropic symmetrization for stable points $\mathbf{u} = \mathbf{u}(\mathbf{v})$**

$$\widetilde{\mathsf{A}}_0(\mathsf{v})\partial_t \mathsf{v} + \sum_{i\in\mathcal{D}} \widetilde{\mathsf{A}}_i(\mathsf{v})\partial_i \mathsf{v} - \sum_{i,j\in\mathcal{D}} \partial_i\big(\widetilde{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{v})\partial_j \mathsf{v}\big) - \sum_{i,j\in\mathcal{D}} \partial_i\big(\widetilde{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{v})\partial_j \mathsf{v}\big) = 0$$

$$\widetilde{\mathsf{A}}_0 = \partial_{\mathsf{v}}\mathsf{u} \quad \widetilde{\mathsf{A}}_i = \mathsf{A}_i\partial_{\mathsf{v}}\mathsf{u} \quad \widetilde{\mathsf{B}}^{\mathrm{d}}_{ij} = \mathsf{B}^{\mathrm{d}}_{ij}\partial_{\mathsf{v}}\mathsf{u} \quad \widetilde{\mathsf{B}}^{\mathrm{c}}_{ij} = \mathsf{B}^{\mathrm{c}}_{ij}\partial_{\mathsf{v}}\mathsf{u} \quad \det \widetilde{\mathsf{A}}_0 = \frac{\rho^2 T^5}{\varkappa}\,\frac{\partial_T \mathcal{E}}{\partial_\rho p}$$

- **Structure of entropic symmetrized system**

$\widetilde{\mathsf{A}}_0$ symmetric positive definite for stable points $\qquad \widetilde{\mathsf{A}}_i$ symmetric for $i \in \mathcal{D}$

$$(\widetilde{\mathsf{B}}^{\mathrm{d}}_{ij})^t = \widetilde{\mathsf{B}}^{\mathrm{d}}_{ji} \qquad \sum_{i,j\in\mathcal{D}} \xi_i\xi_j\widetilde{\mathsf{B}}^{\mathrm{d}}_{ij} \text{ positive semi definite} \qquad (\widetilde{\mathsf{B}}^{\mathrm{c}}_{ij})^t = -\widetilde{\mathsf{B}}^{\mathrm{c}}_{ji}$$

The map $\mathsf{u} \mapsto \mathsf{v}$ is generally not globally invertible

Symmetrized Augmented System (2)

- **Normal variable**

$$\mathsf{w} = \big(\rho, \boldsymbol{w}, \boldsymbol{v}, T\big)^t \quad \mathsf{w} = (\mathsf{w}_{\mathrm{I}}, \mathsf{w}_{\mathrm{II}})^t \quad \mathsf{w}_{\mathrm{I}} = (\rho, \boldsymbol{w})^t \quad \mathsf{w}_{\mathrm{II}} = (\boldsymbol{v}, T)^t$$

$$\mathbb{R}^{\mathsf{n}} = \mathbb{R}^{\mathsf{n}_{\mathrm{I}}} \times \mathbb{R}^{\mathsf{n}_{\mathrm{II}}} \quad \mathsf{n} = \mathsf{n}_{\mathrm{I}} + \mathsf{n}_{\mathrm{II}} \quad \mathsf{n}_{\mathrm{I}} = \mathsf{n}_{\mathrm{II}} = d + 1$$

$$\mathsf{w}_{\mathrm{I}} = (\mathsf{w}_{\mathrm{I}'}, \mathsf{w}_{\mathrm{I}''})^t \quad \mathsf{w}_{\mathrm{I}'} = \rho \quad \mathsf{w}_{\mathrm{I}''} = \boldsymbol{w} \quad \boldsymbol{\nabla} \mathsf{w}_{\mathrm{I}'} = \mathsf{w}_{\mathrm{I}''} \quad \mathsf{w}_{\mathrm{r}} = (\mathsf{w}_{\mathrm{I}'}, \mathsf{w}_{\mathrm{II}})^t$$

$\mathsf{u} \to \mathsf{w}$ diffeomorphism from $\mathcal{O}_{\mathsf{u}}$ onto $\mathcal{O}_{\mathsf{w}} = \mathcal{O}_{\mathsf{z}}$ since $\mathsf{w} = \mathsf{z}$

- **Normal form**

$\mathsf{u} = \mathsf{u}(\mathsf{w})$ and multiplication on the left by $(\partial_{\mathsf{w}} \mathsf{v})^t$

Add $\big(\partial_t \rho + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v})\big) \times \mathsf{m}$ to the first equation   Non conservative form

$$\overline{\mathsf{A}}_0 = (\partial_{\mathsf{w}} \mathsf{v})^t \partial_{\mathsf{w}} \mathsf{u} + \mathsf{m}\, \mathsf{e}_1 \otimes \mathsf{e}_1 \qquad \overline{\mathsf{A}}_i = (\partial_{\mathsf{w}} \mathsf{v})^t \partial_{\mathsf{w}} \mathsf{F}_i + \mathsf{m} v_i\, \mathsf{e}_1 \otimes \mathsf{e}_1 \quad i \in \mathcal{D}$$

$$\overline{\mathsf{A}}_0(\mathsf{w}) \partial_t \mathsf{w} + \sum_{i \in \mathcal{D}} \overline{\mathsf{A}}_i(\mathsf{w}) \partial_i \mathsf{w} - \sum_{i,j \in \mathcal{D}} \overline{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{w}) \partial_i \partial_j \mathsf{w} - \sum_{i,j \in \mathcal{D}} \overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w}) \partial_i \partial_j \mathsf{w} = \mathsf{h}(\mathsf{w}, \boldsymbol{\nabla} \mathsf{w})$$

Symmetrized Augmented System (3)

- **Normal form**

$$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t \mathsf{w} + \sum_{i\in\mathcal{D}} \overline{\mathsf{A}}_i(\mathsf{w})\partial_i \mathsf{w} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{w})\partial_i\partial_j \mathsf{w} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_i\partial_j \mathsf{w} = \mathsf{h}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w})$$

- **Properties of the normal form**

$\overline{\mathsf{A}}_0 = \mathrm{diag}(\overline{\mathsf{A}}_0^{\mathrm{I,I}}, \overline{\mathsf{A}}_0^{\mathrm{II,II}})$ symmetric positive definite $\qquad \overline{\mathsf{A}}_i$ symmetic for $i \in \mathcal{D}$

$(\overline{\mathsf{B}}^{\mathrm{d}}_{ij})^t = \overline{\mathsf{B}}^{\mathrm{d}}_{ji} \qquad \overline{\mathsf{B}}^{\mathrm{d}}_{ij} = \mathrm{diag}(0, \overline{\mathsf{B}}^{\mathrm{d\,II,II}}_{ij}) \qquad \overline{\mathsf{B}}^{\mathrm{d\,II,II}} = \sum_{i,j\in\mathcal{D}} \xi_i\xi_j \overline{\mathsf{B}}^{\mathrm{d\,II,II}}_{ij}$ positive definite

$(\overline{\mathsf{B}}^{\mathrm{c}}_{ij})^t = -\overline{\mathsf{B}}^{\mathrm{c}}_{ji} \qquad \overline{\mathsf{B}}^{\mathrm{c\,I,I}}_{ij} = 0 \qquad \overline{\mathsf{B}}^{\mathrm{c\,I,II}}_{ij},\ \overline{\mathsf{B}}^{\mathrm{c\,II,I}}_{ij},\ \overline{\mathsf{A}}_0^{\mathrm{II,II}}$ depend on $\mathsf{w}_{\mathrm{r}} = (\mathsf{w}_{\mathrm{I'}}, \mathsf{w}_{\mathrm{II}})^t$

- **Right hand side**

$$\mathsf{h} = (\mathsf{h}_{\mathrm{I}}, \mathsf{h}_{\mathrm{II}})^t \qquad \mathsf{h}_{\mathrm{I}} = \Big(-\mathsf{m}\rho\boldsymbol{\nabla\cdot v}, -\frac{\varkappa}{T}\sum_{i\in\mathcal{D}} w_i \boldsymbol{\nabla} v_i\Big)^t \qquad \mathsf{h}_{\mathrm{II}} = \mathsf{h}_{\mathrm{II}}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w})$$

Symmetrized Augmented System (4)

- **Gradient constraint for nonlinear equations**

  Natural equation for $\boldsymbol{w} - \boldsymbol{\nabla}\rho$

  $$\partial_t(\boldsymbol{w} - \boldsymbol{\nabla}\rho) + \boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{\nabla}(\boldsymbol{w} - \boldsymbol{\nabla}\rho) + (\boldsymbol{w} - \boldsymbol{\nabla}\rho)\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t\boldsymbol{\cdot}(\boldsymbol{w} - \boldsymbol{\nabla}\rho) = 0$$

  If w is smooth enough, $\boldsymbol{w}_0 - \boldsymbol{\nabla}\rho_0 = 0$ and $\boldsymbol{w}^\star = 0$ then $\boldsymbol{w} - \boldsymbol{\nabla}\rho = 0$

- **Linearized equation with gradient constraint**

  $$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t\widetilde{\mathsf{w}} + \sum_{i\in\mathcal{D}}\overline{\mathsf{A}}_i(\mathsf{w})\partial_i\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}}\overline{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{w})\partial_i\partial_j\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}}\overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_i\partial_j\widetilde{\mathsf{w}} =$$

  $$\Big(-\mathsf{m}\,\rho\,\boldsymbol{\nabla}\boldsymbol{\cdot}\widetilde{\boldsymbol{v}}, -\sum_{i\in\mathcal{D}}\frac{\varkappa}{T}\widetilde{w}_i\boldsymbol{\nabla}v_i, \mathsf{h}_{\mathrm{II}}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w})\Big)^t$$

Symmetrized Augmented System (5)

- **Linearized equation with gradient constraint**

$$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t\widetilde{\mathsf{w}} + \sum_{i\in\mathcal{D}} \overline{\mathsf{A}}_i'(\mathsf{w})\partial_i\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}_{ij}^{\mathrm{d}}(\mathsf{w})\partial_i\partial_j\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}_{ij}^{\mathrm{c}}(\mathsf{w})\partial_i\partial_j\widetilde{\mathsf{w}}$$

$$+ \overline{\mathsf{L}}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w}_{\mathrm{II}})\widetilde{\mathsf{w}} = \mathsf{h}'(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w}) = \big(0, \mathsf{h}_{\mathrm{II}}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w})\big)^t$$

$$\overline{\mathsf{A}}_i'(\mathsf{w}) = \overline{\mathsf{A}}_i(\mathsf{w}) + \mathsf{m}\rho\mathsf{e}_1\otimes\mathsf{e}_{d+1+i} \qquad \overline{\mathsf{L}}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w}_{\mathrm{II}}) = \sum_{i\in\mathcal{D}} \frac{\varkappa}{T}(0, \boldsymbol{\nabla}v_i, 0_{1,\mathsf{n}_{\mathrm{I}}}, 0)^t\otimes\mathsf{e}_{i+1}$$

- **Gradient constraint for linearized equations**

Natural equation for $\widetilde{\boldsymbol{w}} - \boldsymbol{\nabla}\widetilde{\rho}$

$$\partial_t(\widetilde{\boldsymbol{w}} - \boldsymbol{\nabla}\widetilde{\rho}) + \boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{\nabla}(\widetilde{\boldsymbol{w}} - \boldsymbol{\nabla}\widetilde{\rho}) + (\boldsymbol{w} - \boldsymbol{\nabla}\rho)\,\boldsymbol{\nabla}\boldsymbol{\cdot}\widetilde{\boldsymbol{v}} + \boldsymbol{\nabla}\boldsymbol{v}^t\boldsymbol{\cdot}(\widetilde{\boldsymbol{w}} - \boldsymbol{\nabla}\widetilde{\rho}) = 0$$

If w and $\widetilde{\mathsf{w}}$ are regular, $\boldsymbol{w} - \boldsymbol{\nabla}\rho = 0$, $\widetilde{\boldsymbol{w}}_0 - \boldsymbol{\nabla}\widetilde{\rho}_0 = 0$, $\widetilde{\boldsymbol{w}}^\star = 0$ then $\widetilde{\boldsymbol{w}} - \boldsymbol{\nabla}\widetilde{\rho} = 0$

5 Linearized Estimates

Linearized Equations (1)

- **Linearized equations**

$$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t\widetilde{\mathsf{w}} + \sum_{i\in\mathcal{D}} \overline{\mathsf{A}}_i'(\mathsf{w})\partial_i\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}_{ij}^{\mathrm{d}}(\mathsf{w})\partial_i\partial_j\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}_{ij}^{\mathrm{c}}(\mathsf{w})\partial_i\partial_j\widetilde{\mathsf{w}} + \overline{\mathsf{L}}(\mathsf{w},\nabla\mathsf{w}_{\mathrm{r}})\widetilde{\mathsf{w}} = \mathsf{f}+\mathsf{g}$$

- **Assumptions on the coefficients**

$\overline{\mathsf{A}}_0 = \mathrm{diag}(\overline{\mathsf{A}}_0^{\mathrm{I,I}}, \overline{\mathsf{A}}_0^{\mathrm{II,II}})$ symmetric positive definite block diagonal

$\overline{\mathsf{A}}_i'^{\mathrm{I,I}}$ are symmetric, $(\overline{\mathsf{B}}_{ij}^{\mathrm{d}})^t = \overline{\mathsf{B}}_{ji}^{\mathrm{d}}$, $\overline{\mathsf{B}}_{ij}^{\mathrm{d}} = \mathrm{diag}(0, \overline{\mathsf{B}}_{ij}^{\mathrm{d\,II,II}})$

$\overline{\mathsf{B}}^{\mathrm{d\,II,II}} = \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}_{ij}^{\mathrm{d\,II,II}}\xi_i\xi_j$ is positive definite for $\boldsymbol{\xi} \in \Sigma^{d-1}$

$(\overline{\mathsf{B}}_{ij}^{\mathrm{c}})^t = -\overline{\mathsf{B}}_{ji}^{\mathrm{c}}$ $\quad \overline{\mathsf{B}}_{ij}^{\mathrm{c,I,I}} = 0$ $\quad \overline{\mathsf{A}}_0^{\mathrm{II,II}}, \overline{\mathsf{B}}_{ij}^{\mathrm{c,I,II}}, \overline{\mathsf{B}}_{ij}^{\mathrm{c,II,I}}$ only depend on $\mathsf{w}_{\mathrm{r}} = (\mathsf{w}_{\mathrm{I'}}, \mathsf{w}_{\mathrm{II}})^t$

$\overline{\mathsf{L}} = \mathrm{diag}(\overline{\mathsf{L}}^{\mathrm{I,I}}, \overline{\mathsf{L}}^{\mathrm{II,II}})$ $\quad \overline{\mathsf{L}}^{\mathrm{I,I}} = \mathfrak{L}^{\mathrm{I,I}}(\mathsf{w})\boldsymbol{\nabla}\mathsf{w}_{\mathrm{r}}$ $\quad \overline{\mathsf{L}}^{\mathrm{II,II}} = \mathfrak{L}^{\mathrm{II,II}}(\mathsf{w})\boldsymbol{\nabla}\mathsf{w}_{\mathrm{r}}$

$\overline{\mathsf{A}}_0, \overline{\mathsf{A}}_i', \overline{\mathsf{B}}_{ij}^{\mathrm{d}}, \overline{\mathsf{B}}_{ij}^{\mathrm{c}}, \mathfrak{L}^{\mathrm{I,I}}, \mathfrak{L}^{\mathrm{II,II}}$ are C^{l+2} over $\mathcal{O}_{\mathsf{w}}$ $\qquad \overline{\mathsf{L}}(\mathsf{w},\nabla\mathsf{w}_{\mathrm{r}})\,\widetilde{\mathsf{w}}^\star = 0$

Linearized Equations (2)

- **Assumptions on w**

  $d \geq 1 \quad l \geq l_0 + 2$ where $l_0 = [d/2] + 1 \quad 1 \leq l' \leq l$

  w given function of $(t, \boldsymbol{x})$ over $[0, \bar{\tau}] \times \mathbb{R}^d$ with $\bar{\tau} > 0$

$$\begin{cases} \mathsf{w}_{\mathrm{I}} - \mathsf{w}_{\mathrm{I}}^{\star} \in C^0\big([0,\bar{\tau}], H^l\big) \cap C^1\big([0,\bar{\tau}], H^{l-2}\big) \\ \mathsf{w}_{\mathrm{II}} - \mathsf{w}_{\mathrm{II}}^{\star} \in C^0\big([0,\bar{\tau}], H^l\big) \cap C^1\big([0,\bar{\tau}], H^{l-2}\big) \cap L^2\big((0,\bar{\tau}), H^{l+1}\big) \end{cases}$$

  $\mathcal{O}_0 \subset \overline{\mathcal{O}}_0 \subset \mathcal{O}_{\mathsf{w}},\ 0 < a_1 < \mathrm{dist}(\overline{\mathcal{O}}_0, \partial\mathcal{O}_{\mathsf{w}}),\ \ \mathcal{O}_1 = \{\, \mathsf{w} \in \mathcal{O}_{\mathsf{w}};\ \mathrm{dist}(\mathsf{w}, \overline{\mathcal{O}}_0) < a_1 \,\}$

  $\mathsf{w}_0(\boldsymbol{x}) = \mathsf{w}(0, \boldsymbol{x}) \in \mathcal{O}_0,\ \mathsf{w}(t, \boldsymbol{x}) \in \mathcal{O}_1,\ (t, \boldsymbol{x}) \in [0, \bar{\tau}] \times \mathbb{R}^d$

- **Assumptions on f and g**

  f and g given functions of $(t, \boldsymbol{x})$ over $[0, \bar{\tau}] \times \mathbb{R}^d \qquad 1 \leq l' \leq l$

  $\mathsf{f} \in C^0\big([0,\bar{\tau}], H^{l'-1}\big) \cap L^1\big((0,\bar{\tau}), H^{l'}\big) \qquad \mathsf{g} \in C^0\big([0,\bar{\tau}], H^{l'-1}\big) \quad \mathsf{g}_{\mathrm{I}} = 0$

Linearized Equations (3)

- **Assumptions on $\widetilde{\mathsf{w}}$**

$$\widetilde{\mathsf{w}}_{\rm I} - \widetilde{\mathsf{w}}_{\rm I}^\star \in C^0\big([0,\bar\tau], H^{l'}\big) \cap C^1\big([0,\bar\tau], H^{l'-2}\big),$$

$$\widetilde{\mathsf{w}}_{\rm II} - \widetilde{\mathsf{w}}_{\rm II}^\star \in C^0\big([0,\bar\tau], H^{l'}\big) \cap C^1\big([0,\bar\tau], H^{l'-2}\big) \cap L^2\big((0,\bar\tau), H^{l'+1}\big),$$

- **Bounding quantities**

$$M^2 = \sup_{0\le\tau\le\bar\tau} |\mathsf{w}(\tau) - \mathsf{w}^\star|_l^2, \qquad M_{\rm t}^2 = \int_0^{\bar\tau} |\partial_t \mathsf{w}(\tau)|_{l-2}^2 \, d\tau, \qquad M_{\rm r}^2 = \int_0^{\bar\tau} |\nabla \mathsf{w}_{\rm r}(\tau)|_l^2 \, d\tau$$

- **Linearized estimates for $1 \le l' \le l$**

There exists constants $\mathsf{c}_1(\mathcal{O}_1) \ge 1$ and $\mathsf{c}_2(\mathcal{O}_1, M) \ge 1$ increasing with M with

$$\sup_{0\le\tau\le t} |\widetilde{\mathsf{w}}(\tau) - \widetilde{\mathsf{w}}^\star|_{l'}^2 + \int_0^t |\widetilde{\mathsf{w}}_{\rm II}(\tau) - \widetilde{\mathsf{w}}_{\rm II}^\star|_{l'+1}^2 \, d\tau \le \ \mathsf{c}_1^2 \exp\Big(\mathsf{c}_2\big(t + M_{\rm t}\sqrt{t} + M_{\rm r}\sqrt{t}\,\big)\Big)\times$$

$$\Big(|\widetilde{\mathsf{w}}_0 - \widetilde{\mathsf{w}}^\star|_{l'}^2 + \mathsf{c}_2\Big\{\int_0^t |\mathsf{f}|_{l'} \, d\tau\Big\}^2 + \mathsf{c}_2 \int_0^t |\mathsf{g}_{\rm II}|_{l'-1}^2 \, d\tau\Big)$$

Linearized Equations (4)

- **Sketch of the proof for the linearized estimates**

  Notation $\delta\widetilde{\mathsf{w}} = \widetilde{\mathsf{w}} - \widetilde{\mathsf{w}}^\star$ and $E_k^2(\phi) = \sum_{0\le|\alpha|\le k} \frac{|\alpha|!}{\alpha!} \int_{\mathbb{R}^d} \langle\, \overline{\mathsf{A}}_0(\mathsf{w})\partial^\alpha\phi, \partial^\alpha\phi\rangle\, d\boldsymbol{x}$

  Use of Gronwall Lemma and the inequality ($\delta(\mathcal{O}_1) \le 1$ small constant)

$$\partial_t E_{l'}^2(\delta\widetilde{\mathsf{w}}) + \delta_1|\delta\widetilde{\mathsf{w}}_{\mathrm{II}}|_{l'+1}^2 \le \mathsf{c}_2\big(1 + |\partial_t\mathsf{w}|_{l-2} + |\nabla\mathsf{w}_{\mathrm{r}}|_l\big)E_{l'}^2(\delta\widetilde{\mathsf{w}})$$

$$+ \mathsf{c}_2|\mathsf{f}|_{l'}E_{l'}(\delta\widetilde{\mathsf{w}}) + \mathsf{c}_2|\mathsf{g}_{\mathrm{II}}|_{l'-1}^2$$

- **Zeroth order inequality $k = 0$**

  ⋆ Multiply the equation by $\delta\widetilde{\mathsf{w}}$ and integrate over $\mathbb{R}^d$

  ⋆ Time derivative terms estimated with the symmetry of $\overline{\mathsf{A}}_0$

$$\langle\delta\widetilde{\mathsf{w}}, \overline{\mathsf{A}}_0(\mathsf{w})\partial_t\delta\widetilde{\mathsf{w}}\rangle = \tfrac{1}{2}\partial_t\langle\delta\widetilde{\mathsf{w}}, \overline{\mathsf{A}}_0(\mathsf{w})\delta\widetilde{\mathsf{w}}\rangle - \tfrac{1}{2}\langle\delta\widetilde{\mathsf{w}}, \partial_t\overline{\mathsf{A}}_0(\mathsf{w})\delta\widetilde{\mathsf{w}}\rangle,$$

  $\partial_t\overline{\mathsf{A}}_0(\mathsf{w}) = \partial_{\mathsf{w}}\overline{\mathsf{A}}_0\,\partial_t\mathsf{w}$ is estimated with $|\partial_t\overline{\mathsf{A}}_0|_{L^\infty} \le \mathsf{c}_0|\partial_t\overline{\mathsf{A}}_0|_{l-2} \le \mathsf{c}_1|\partial_t\mathsf{w}|_{l-2}$

Linearized Equations (5)

- **Zeroth order inequality $k = 0$ (continued)**
  - ⋆ The products $\langle \delta\widetilde{\mathsf{w}}, \overline{\mathsf{A}}'_i(\mathsf{w})\partial_i\delta\widetilde{\mathsf{w}}\rangle$ are evaluated by blocks

    Symmetry for the (I, I) terms, direct estimates for (I, II) and (II, II) terms

    The (II, I) terms are integrated by parts, $|\overline{\mathsf{A}}_i|_{L^\infty} \leq \mathsf{c}_1$ and $|\partial_i\overline{\mathsf{A}}_i|_{L^\infty} \leq \mathsf{c}_2$
  - ⋆ Dissipative terms integrated by parts, $|\partial_i\overline{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{w})|_{L^\infty} \leq \mathsf{c}_2$, Garding inequality

$$\delta_1|\phi_{\mathrm{II}}|_1^2 \leq \sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle \overline{\mathsf{B}}^{\mathrm{d}\,\mathrm{II},\mathrm{II}}_{ij}(\mathsf{w})\partial_j\phi_{\mathrm{II}}, \partial_i\phi_{\mathrm{II}}\rangle\, d\boldsymbol{x} + \mathsf{c}_2|\phi_{\mathrm{II}}|_0^2 \qquad \phi_{\mathrm{II}} \in H^1(\mathbb{R}^d)$$

  - ⋆ Antisymmetric terms integrated by parts and the first sum vanishes

$$-\sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle \delta\widetilde{\mathsf{w}}, \overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_i\partial_j\delta\widetilde{\mathsf{w}}\rangle\, d\boldsymbol{x} = \sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle \partial_i\delta\widetilde{\mathsf{w}}, \overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_j\delta\widetilde{\mathsf{w}}\rangle\, d\boldsymbol{x}$$

$$+ \sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle \delta\widetilde{\mathsf{w}}, \partial_i\overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_j\delta\widetilde{\mathsf{w}}\rangle\, d\boldsymbol{x}.$$

Linearized Equations (6)

- **Zeroth order inequality $k = 0$ (continued)**
  - ⋆ Block evaluation of the terms $\sum_{i,j\in\mathcal{D}}\int_{\mathbb{R}^d}\langle\delta\widetilde{\mathsf{w}},\partial_i\overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_j\delta\widetilde{\mathsf{w}}\rangle\,d\boldsymbol{x}$
    The terms (I, I), (I, II), (II, II) easily estimated, (II, I) terms integrated by parts and use of Use of $|\partial_i\partial_j\overline{\mathsf{B}}^{\mathrm{c\,II,I}}_{ij}|\le \mathsf{c}_2$ since $l\ge l_0+2$

$$\sum_{i,j\in\mathcal{D}}\int_{\mathbb{R}^d}\langle\delta\widetilde{\mathsf{w}}_{\mathrm{II}},\partial_i\overline{\mathsf{B}}^{\mathrm{c\,II,I}}_{ij}(\mathsf{w})\partial_j\delta\widetilde{\mathsf{w}}_{\mathrm{I}}\rangle\,d\boldsymbol{x} = -\sum_{i,j\in\mathcal{D}}\int_{\mathbb{R}^d}\langle\partial_j\delta\widetilde{\mathsf{w}}_{\mathrm{II}},\partial_i\overline{\mathsf{B}}^{\mathrm{c\,II,I}}_{ij}(\mathsf{w})\delta\widetilde{\mathsf{w}}_{\mathrm{I}}\rangle\,d\boldsymbol{x}$$
$$-\sum_{i,j\in\mathcal{D}}\int_{\mathbb{R}^d}\langle\delta\widetilde{\mathsf{w}}_{\mathrm{II}},\partial_i\partial_j\overline{\mathsf{B}}^{\mathrm{c\,II,I}}_{ij}(\mathsf{w})\delta\widetilde{\mathsf{w}}_{\mathrm{I}}\rangle\,d\boldsymbol{x}.$$

  - ⋆ Zeroth order terms $\int_{\mathbb{R}^d}\langle\delta\widetilde{\mathsf{w}},\overline{\mathsf{L}}(\mathsf{w},\nabla\mathsf{w}_{\mathrm{r}})\delta\widetilde{\mathsf{w}}\rangle\,d\boldsymbol{x}\le\mathsf{c}_2|\delta\widetilde{\mathsf{w}}|_0^2$ and right hand side terms $\int_{\mathbb{R}^d}\langle\delta\widetilde{\mathsf{w}},\mathsf{f}\rangle\,d\boldsymbol{x}\le\mathsf{c}_1|\delta\widetilde{\mathsf{w}}|_0|\mathsf{f}|_0$ and $\int_{\mathbb{R}^d}\langle\delta\widetilde{\mathsf{w}},\mathsf{g}\rangle\,d\boldsymbol{x}\le|\delta\widetilde{\mathsf{w}}|_0|\mathsf{g}|_0$

$$\partial_t E_0^2(\delta\widetilde{\mathsf{w}})+\delta_1|\delta\widetilde{\mathsf{w}}_{\mathrm{II}}|_1^2\le\mathsf{c}_1|\mathsf{f}|_0|\delta\widetilde{\mathsf{w}}|_0+\mathsf{c}_1|\mathsf{g}_{\mathrm{II}}|_0^2+\mathsf{c}_2(1+|\partial_t\mathsf{w}|_{l-2})E_0^2(\delta\widetilde{\mathsf{w}}).$$

Linearized Equations (7)

- **The l'th order inequality**

  ⋆ The l'th order inequality obtained from

$$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t\partial^\alpha\widetilde{\mathsf{w}} + \sum_{i\in\mathcal{D}}\overline{\mathsf{A}}'_i(\mathsf{w})\partial_i\partial^\alpha\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}}\overline{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{w})\partial_i\partial_i\partial^\alpha\widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}}\overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\partial_i\partial_i\partial^\alpha\widetilde{\mathsf{w}} + \overline{\mathsf{L}}(\mathsf{w},\nabla\mathsf{w})\partial^\alpha\widetilde{\mathsf{w}} = \mathsf{h}^\alpha$$

$$\mathsf{h}^\alpha = \overline{\mathsf{A}}_0\partial^\alpha\big(\overline{\mathsf{A}}_0^{-1}\mathsf{f}\big) + \overline{\mathsf{A}}_0\partial^\alpha\big(\overline{\mathsf{A}}_0^{-1}\mathsf{g}\big) - \sum_{i\in\mathcal{D}}\overline{\mathsf{A}}_0\big[\partial^\alpha,\overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{A}}'_i\big]\partial_i\widetilde{\mathsf{w}} - \overline{\mathsf{A}}_0\big[\partial^\alpha,\overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{L}}\,\big]\widetilde{\mathsf{w}}$$

$$+ \sum_{i,j\in\mathcal{D}}\overline{\mathsf{A}}_0\big[\partial^\alpha,\overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{B}}^{\mathrm{d}}_{ij}\big]\partial_i\partial_j\widetilde{\mathsf{w}} + \sum_{i,j\in\mathcal{D}}\overline{\mathsf{A}}_0\big[\partial^\alpha,\overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{B}}^{\mathrm{c}}_{ij}\big]\partial_i\partial_j\widetilde{\mathsf{w}}.$$

  Multiply by $\partial^\alpha\delta\widetilde{\mathsf{w}}$, myltiply by $|\alpha|!/\alpha!$, integrate over $\mathbb{R}^d$, sum over $1 \le |\alpha| \le l'$, and add zeroth order estimate

Linearized Equations (8)

- **The l'th order inequality**
  - ⋆ Proceeding as for the zeroth order estimaet and use of $|\delta\widetilde{\mathsf{w}}|_{l'} \leq \mathsf{c}_1 E_{l'}(\delta\widetilde{\mathsf{w}})$

$$\partial_t E_{l'}^2(\delta\widetilde{\mathsf{w}}) + \delta_1|\delta\widetilde{\mathsf{w}}_{\text{II}}|_{l'+1}^2 \leq \mathsf{c}_2(1+|\partial_t \mathsf{w}|_{l-2})E_{l'}^2(\delta\widetilde{\mathsf{w}}) + \sum_{0\leq|\alpha|\leq l'} \frac{|\alpha|!}{\alpha!}\int_{\mathbb{R}^d} \langle \mathsf{h}^\alpha, \partial^\alpha \delta\widetilde{\mathsf{w}}\rangle\, d\boldsymbol{x}$$

  - ⋆ Right hand sides with $|\overline{\mathsf{A}}_0^{-1}\mathsf{f}|_{l'} \leq \mathsf{c}_1\big(1+|\overline{\mathsf{A}}_0^{-1}(\mathsf{w})-\overline{\mathsf{A}}_0^{-1}(\mathsf{w}^\star)|_l\big)\,|\mathsf{f}|_{l'} \leq \mathsf{c}_2|\mathsf{f}|_{l'}$ and eventual integration by parts for g

$$\Big|\int_{\mathbb{R}^d}\langle \overline{\mathsf{A}}_0\partial^\alpha\big(\overline{\mathsf{A}}_0^{-1}\mathsf{f}\big), \partial^\alpha\delta\widetilde{\mathsf{w}}\rangle\, d\boldsymbol{x}\Big| \leq |\overline{\mathsf{A}}_0|_\infty\, |\overline{\mathsf{A}}_0^{-1}\mathsf{f}|_{l'}\, |\delta\widetilde{\mathsf{w}}|_{l'} \leq \mathsf{c}_2|\mathsf{f}|_{l'}\, |\delta\widetilde{\mathsf{w}}|_{l'}$$

$$\Big|\int_{\mathbb{R}^d}\langle \overline{\mathsf{A}}_0\partial^\alpha\big(\overline{\mathsf{A}}_0^{-1}\mathsf{g}\big), \partial^\alpha\delta\widetilde{\mathsf{w}}\rangle\, d\boldsymbol{x}\Big| \leq \mathsf{c}_2|\mathsf{g}_{\text{II}}|_{l'-1}\, |\delta\widetilde{\mathsf{w}}_{\text{II}}|_{l'+1}$$

Linearized Equations (9)

- **The l'th order inequality**

  ⋆ Convective and dissipative contributions using commutator estimates

$$\Big|\int_{\mathbb{R}^d}\big\langle \overline{\mathsf{A}}_0\big[\partial^\alpha, \overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{A}}_i'\big]\partial_i\widetilde{\mathsf{w}}, \partial^\alpha\delta\widetilde{\mathsf{w}}\big\rangle\,d\boldsymbol{x}\Big| \le \mathsf{c}_2|\delta\widetilde{\mathsf{w}}|_{l'}^2$$

$$\Big|\int_{\mathbb{R}^d}\big\langle \overline{\mathsf{A}}_0\big[\partial^\alpha, \overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{B}}_{ij}^{\mathrm{d}}\big]\partial_i\partial_j\widetilde{\mathsf{w}}, \partial^\alpha\delta\widetilde{\mathsf{w}}\big\rangle\,d\boldsymbol{x}\Big| \le \mathsf{c}_2\,|\delta\widetilde{\mathsf{w}}_{\mathrm{II}}|_{l'+1}\,|\delta\widetilde{\mathsf{w}}_{\mathrm{II}}|_{l'}$$

$$\sum_{0\le|\alpha|\le l'}\big|[\partial^\alpha, u]v\big|_0 \le \mathsf{c}_0|\nabla u|_{\bar{l}-1}|v|_{l'-1} \qquad \nabla u\in H^{\bar{l}-1}\quad v\in H^{l'-1}\quad \bar{l}\ge l_0+1$$

  ⋆ Block evaluation for the antisymmetric terms. The (I,I) terms vanish and the (I,II) and $(\mathrm{II},\mathrm{II})$ are estimated with the commutator estimates

$$-\sum_{i,j\in\mathcal{D}}\int_{\mathbb{R}^d}\big\langle \overline{\mathsf{A}}_0\big[\partial^\alpha, (\overline{\mathsf{A}}_0)^{-1}\,\overline{\mathsf{B}}_{ij}^{\mathrm{c}}\big]\partial_i\partial_j\delta\widetilde{\mathsf{w}}, \partial^\alpha\delta\widetilde{\mathsf{w}}\big\rangle\,d\boldsymbol{x}$$

Linearized Equations (10)

- **The l'th order inequality**
  - ⋆ The $(\textsc{ii},\textsc{i})$ antisymmetric terms with $[\partial^\alpha, \mathfrak{V}]\partial_i\phi = \partial_i([\partial^\alpha,\mathfrak{V}]\phi) - [\partial^\alpha, \partial_i\mathfrak{V}]\phi$ are integration by parts

$$- \sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle \overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}} [\partial^\alpha, (\overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}})^{-1}\, \overline{\mathsf{B}}_{ij}^{\mathrm{c}\,\textsc{ii},\textsc{i}}]\partial_i\partial_j\delta\widetilde{\mathsf{w}}_{\textsc{i}}, \partial^\alpha\delta\widetilde{\mathsf{w}}_{\textsc{ii}}\rangle\, d\boldsymbol{x} =$$

$$\sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle [\partial^\alpha, (\overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}})^{-1}\, \overline{\mathsf{B}}_{ij}^{\mathrm{c}\,\textsc{ii},\textsc{i}}]\partial_j\delta\widetilde{\mathsf{w}}_{\textsc{i}}, \partial_i(\overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}}\partial^\alpha\delta\widetilde{\mathsf{w}}_{\textsc{ii}})\rangle\, d\boldsymbol{x}$$

$$+ \sum_{i,j\in\mathcal{D}} \int_{\mathbb{R}^d} \langle \overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}} [\partial^\alpha, \partial_i((\overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}})^{-1}\, \overline{\mathsf{B}}_{ij}^{\mathrm{c}\,\textsc{ii},\textsc{i}})]\partial_j\delta\widetilde{\mathsf{w}}_{\textsc{i}}, \partial^\alpha\delta\widetilde{\mathsf{w}}_{\textsc{ii}}\rangle\, d\boldsymbol{x}$$

Last sum estimated by using that $(\overline{\mathsf{A}}_0^{\textsc{ii},\textsc{ii}})^{-1}\, \overline{\mathsf{B}}_{ij}^{\mathrm{c}\,\textsc{ii},\textsc{i}}$ only depends on w_{r}

Upper bounds in the form $\mathsf{c}_2|\delta\widetilde{\mathsf{w}}|_{l'}\,|\delta\widetilde{\mathsf{w}}_{\textsc{ii}}|_{l'+1} + \mathsf{c}_2|\nabla\mathsf{w}_{\mathrm{r}}|_l|\delta\widetilde{\mathsf{w}}|_{l'}^2$

Linearized Equations (11)

- **The l'th order inequality**
  - ⋆ Terms associated with $\overline{\mathsf{A}}_0\big[\partial^\alpha, \overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{L}}\,\big]\widetilde{\mathsf{w}}$ estimated as

$$\left|\int_{\mathbb{R}^d}\big\langle\overline{\mathsf{A}}_0\big[\partial^\alpha, \overline{\mathsf{A}}_0^{-1}\,\overline{\mathsf{L}}\,\big]\widetilde{\mathsf{w}}, \partial^\alpha\delta\widetilde{\mathsf{w}}\big\rangle\, d\boldsymbol{x}\right| \le \mathsf{c}_2|\nabla\mathsf{w}_{\mathrm{r}}|_l|\delta\widetilde{\mathsf{w}}|_{l'}^2$$

    since $\overline{\mathsf{L}} = \mathrm{diag}(\,\overline{\mathsf{L}}^{\mathrm{I,I}}, \overline{\mathsf{L}}^{\mathrm{II,II}}\,)$ is a linear function of $\nabla\mathsf{w}_{\mathrm{r}}$
  - ⋆ Final differential inequality

$$\partial_t E_{l'}^2(\delta\widetilde{\mathsf{w}}) + \delta_1|\delta\widetilde{\mathsf{w}}_{\mathrm{II}}|_{l'+1}^2 \le \mathsf{c}_2\big(1 + |\partial_t\mathsf{w}|_{l-2} + |\nabla\mathsf{w}_{\mathrm{r}}|_l\big)E_{l'}^2(\delta\widetilde{\mathsf{w}})$$
$$+\, \mathsf{c}_2|\mathsf{f}|_{l'}E_{l'}(\delta\widetilde{\mathsf{w}}) + \mathsf{c}_2|\mathsf{g}_{\mathrm{II}}|_{l'-1}^2$$

  - ⋆ Apply Gronwall Lemma

Linearized Equations (12)

- **Regularized operators for $0 < \epsilon \leq 1$**

$$\mathsf{R}_\epsilon \phi(\mathbf{r}) = \int \mathfrak{a}_\epsilon(\mathbf{r} - \hat{\mathbf{r}})\phi(\hat{\mathbf{r}})\ d\hat{\mathbf{r}} \quad \mathfrak{a}_\epsilon = \epsilon^{-d}\mathfrak{a}(\mathbf{r}/\epsilon) \quad \int \mathfrak{a}\ d\mathbf{r} = 1 \quad \mathfrak{a} > 0 \text{ on Ball}(0,1)$$

- **Regularized equations**

$$\overline{\mathsf{A}}_0(\mathsf{w})\partial_t \widetilde{\mathsf{w}} + \sum_{i\in\mathcal{D}} \overline{\mathsf{A}}'_i(\mathsf{w})\partial_i \widetilde{\mathsf{w}} - \sum_{i,j\in\mathcal{D}} \overline{\mathsf{B}}^{\mathrm{d}}_{ij}(\mathsf{w})\partial_i\partial_j \widetilde{\mathsf{w}}$$
$$- \sum_{i,j\in\mathcal{D}} \mathsf{R}_\epsilon \overline{\mathsf{B}}^{\mathrm{c}}_{ij}(\mathsf{w})\mathsf{R}_\epsilon \partial_i\partial_j \widetilde{\mathsf{w}} + \overline{\mathsf{L}}(\mathsf{w}, \nabla \mathsf{w}_{\mathrm{r}})\widetilde{\mathsf{w}} = \mathsf{f} + \mathsf{g}$$

- **Existence of solutions for linearized equations**

  Existence for regularized equations for ϵ fixed by uncoupling

  New estimates for solutions of regularized equations independent of ϵ

  Taking the limit $\epsilon \to 0$

6 Existence of Solutions

Existence Results for Diffuse Interface Models

- **Isothermal**

  Hattori and Li (1996) Danchin and Desjardins (2001) Kotschote (2008)
  Bresch et al. (2003) (2019)

- **Euler-Korteweg**

  Bresch et al. (2008) (2019) Benzoni et al. (2005) (2006) (2007)
  Donatelli et al. (2004) (2014) Tzavaras et al. (2018) (2017)

- **Full model**

  Haspot (2009) Kotschote (2012) (2014)

- **Symmetrization for diffuse interface fluids**

  Gavrilyuk and Gouin (2000) Kawashima et al. (2022)

Existence of Strong Solutions (1)

- **Structural assumptions**

  Augmented system in normal form with the gradient constraint

  Linearized equations enforcing the gradient constraint

$$\big(\overline{\mathsf{A}}'_i(\mathsf{w}) - \overline{\mathsf{A}}_i(\mathsf{w})\big)\boldsymbol{\nabla}\mathsf{w} + \overline{\mathsf{L}}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w}_{\mathrm{r}})\mathsf{w} + \mathsf{h}(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w}) = \mathsf{h}'(\mathsf{w}, \boldsymbol{\nabla}\mathsf{w})$$

  Right hand sides in the form

$$\mathsf{h}_{\mathrm{I}} = \sum_{i\in\mathcal{D}} \overline{\mathrm{M}}_i^{\mathrm{I}}(\mathsf{w})\partial_i\mathsf{w}_{\mathrm{r}} + \sum_{i,j\in\mathcal{D}} \overline{\mathrm{M}}_{ij}^{\mathrm{I},\mathrm{I}}(\mathsf{w})\partial_i\mathsf{w}_{\mathrm{r}}\partial_j\mathsf{w}_{\mathrm{r}}$$

$$\mathsf{h}_{\mathrm{II}} = \sum_{i\in\mathcal{D}} \overline{\mathrm{M}}_i^{\mathrm{II}}(\mathsf{w})\partial_i\mathsf{w} + \sum_{i,j\in\mathcal{D}} \overline{\mathrm{M}}_{ij}^{\mathrm{II},\mathrm{II}}(\mathsf{w})\partial_i\mathsf{w}\partial_j\mathsf{w}$$

  w_{r} is the more regular part $\mathsf{w}_{\mathrm{r}} = (\mathsf{w}_{\mathrm{I}'}, \mathsf{w}_{\mathrm{II}})^t$ of the normal vartiable

Existence of Strong Solutions (2)

Theorem 4. *Let* $d \geq 1$, $l \geq l_0 + 2$, $l_0 = [d/2] + 1$, *and let* $b > 0$. *Let* $\mathcal{O}_0 \subset \overline{\mathcal{O}}_0 \subset \mathcal{O}_{\mathsf{w}}$, $0 < a_1 < \operatorname{dist}(\overline{\mathcal{O}}_0, \partial\mathcal{O}_{\mathsf{w}})$, $\mathcal{O}_1 = \{\, \mathsf{w} \in \mathcal{O}_{\mathsf{w}}; \operatorname{dist}(\mathsf{w}, \overline{\mathcal{O}}_0) < a_1 \,\}$. *There exists* $\bar{\tau}(\mathcal{O}_1, b) > 0$ *such that for any* w_0 *with* $\mathsf{w}_0 \in \mathcal{O}_0$, $\mathsf{w}_0 - \mathsf{w}^\star \in H^l$, $\mathsf{w}_{0\mathrm{I}''} = \nabla \mathsf{w}_{0\mathrm{I}'}$ *and*

$$|\mathsf{w}_0 - \mathsf{w}^\star|_l^2 < b^2,$$

there exists a unique local solution w *with initial condition* $\mathsf{w}(0, \boldsymbol{x}) = \mathsf{w}_0(\boldsymbol{x})$, *such that* $\mathsf{w}(t, \boldsymbol{x}) \in \mathcal{O}_1$ *for* $(t, \boldsymbol{x}) \in [0, \bar{\tau}] \times \mathbb{R}^d$, $\mathsf{w}_{\mathrm{I}''} = \nabla \mathsf{w}_{\mathrm{I}'}$, *and*

$$\mathsf{w}_{\mathrm{I}} - \mathsf{w}_{\mathrm{I}}^\star \in C^0\big([0, \bar{\tau}], H^l\big) \cap C^1\big([0, \bar{\tau}], H^{l-2}\big)$$

$$\mathsf{w}_{\mathrm{II}} - \mathsf{w}_{\mathrm{II}}^\star \in C^0\big([0, \bar{\tau}], H^l\big) \cap C^1\big([0, \bar{\tau}], H^{l-2}\big) \cap L^2\big((0, \bar{\tau}), H^{l+1}\big)$$

Moreover, there exists $\mathsf{c}_{\mathrm{loc}}(\mathcal{O}_1, b) \geq 1$ *such that*

$$\sup_{0 \leq \tau \leq \bar{\tau}} |\mathsf{w}(\tau) - \mathsf{w}^\star|_l^2 + \int_0^{\bar{\tau}} |\mathsf{w}_{\mathrm{II}}(\tau) - \mathsf{w}_{\mathrm{II}}^\star|_{l+1}^2 d\tau \leq \mathsf{c}_{\mathrm{loc}}^2 |\mathsf{w}_0 - \mathsf{w}^\star|_l^2.$$

Existence of Strong Solutions (3)

- **Sketch of the proof (1)**

  ⋆ $\mathsf{X}^l_{\bar\tau}\big(\mathcal{O}_1, \overline{M}\,\big)$ defined by $\mathsf{w}-\mathsf{w}^\star \in C^0\big([0,\bar\tau], H^l\big)$, $\partial_t \mathsf{w} \in C^0\big([0,\bar\tau], H^{l-2}\big)$, $\mathsf{w}_{\rm II}-\mathsf{w}^\star_{\rm II} \in L^2\big((0,\bar\tau), H^{l+1}\big)$, $\mathsf{w}(t,\boldsymbol{x}) \in \mathcal{O}_1$, $\mathsf{w}_{\rm I''} = \nabla \mathsf{w}_{\rm I'}$, and

$$\sup_{0\le\tau\le\bar\tau} |\mathsf{w}(\tau)-\mathsf{w}^\star|_l^2 + \int_0^{\bar\tau} |\mathsf{w}_{\rm II}(\tau)-\mathsf{w}^\star_{\rm II}|^2_{l+1}\, d\tau \le \overline{M}^{\,2}$$

$$\int_0^{\bar\tau} |\partial_t \mathsf{w}(\tau)|^2_{l-2}\, d\tau \le \overline{M}^{\,2} \qquad \int_0^{\bar\tau} |\nabla \mathsf{w}_{\rm r}(\tau)|^2_l\, d\tau \le \overline{M}^{\,2}$$

  ⋆ $\mathsf{X}^l_{\bar\tau}\big(\mathcal{O}_1, \overline{M}\,\big)$ invariant by the map $\mathsf{w} \mapsto \widetilde{\mathsf{w}}$ for suitable $\overline{M}$ and $\bar\tau$ small enough

  Rely on a priori estimates for linearized equations applied to $\widetilde{\mathsf{w}}^k$

  Successive approximations $\{\mathsf{w}^k\}_{k\ge 0}$ with $\mathsf{w}^0 = \mathsf{w}^\star$, $\mathsf{w}^{k+1} = \widetilde{\mathsf{w}}^k$ well defined

Existence of Strong Solutions (4)

- **Sketch of the proof (2)**

  ⋆ The sequence $\{\mathsf{w}^k\}_{k\geq 0}$ is convergent over $[0,\bar\tau]$ for the norm

$$\sup_{0\leq\tau\leq\bar\tau} |\delta\widetilde{\mathsf{w}}(\tau)|^2_{l-2} + \int_0^{\bar\tau} |\delta\widetilde{\mathsf{w}}_{\mathrm{II}}(\tau)|^2_{l-1}\, d\tau$$

  Rely on a priori estimates for linearized equations applied to $\mathsf{w}^{k+1} - \mathsf{w}^{k+1}$

  ⋆ $\mathsf{w}^k \to \overline{\mathsf{w}} \in C^0\big([0,\bar\tau], H^{l-2}\big)$ that is a solution (fixed point)

  $\overline{\mathsf{w}} \in L^\infty\big((0,\bar\tau), H^l\big)$ and $\overline{\mathsf{w}}_{\mathrm{II}} - \mathsf{w}^\star_{\mathrm{II}} \in L^2\big((0,\bar\tau), H^{l+1}\big)$

  ⋆ $\overline{\mathsf{w}} \in C^0\big((0,\bar\tau), H^l\big)$ since the sequence

$$\mathsf{w}^\delta = \mathsf{R}_\delta \overline{\mathsf{w}}$$

  form a Cauchy sequence in $C^0\big([0,\bar\tau], H^l\big)$

Existence of Strong Solutions (5)

- **Application to diffuse interface fluids**

Theorem 5. *Let* $d \geq 1$*,* $l \geq l_0 + 2$*, and* $b > 0$*. There exists* $\bar{\tau}(\mathcal{O}_1, b) > 0$ *such that for any* w_0 *with* $\mathsf{w}_0 \in \overline{\mathcal{O}}_0$*,* $\mathsf{w}_0 - \mathsf{w}^\star \in H^l$*,* $\boldsymbol{w}_0 = \boldsymbol{\nabla}\rho_0$ *and* $|\mathsf{w}_0 - \mathsf{w}^\star|_l^2 < b^2$ *there exists a unique local solution* w *with* $\mathsf{w}(0, \boldsymbol{x}) = \mathsf{w}_0(\boldsymbol{x})$*,* $\mathsf{w}(t, \boldsymbol{x}) \in \mathcal{O}_1$*,* $\boldsymbol{w} = \boldsymbol{\nabla}\rho$*, and*

$$\rho - \rho^\star \in C^0\big([0, \bar{\tau}], H^{l+1}\big),$$

$$\boldsymbol{v} - \boldsymbol{v}^\star \in C^0\big([0, \bar{\tau}], H^l\big) \cap L^2\big((0, \bar{\tau}), H^{l+1}\big)$$

$$T - T^\star \in C^0\big([0, \bar{\tau}], H^l\big) \cap L^2\big((0, \bar{\tau}), H^{l+1}\big).$$

Moreover, there exists $\mathsf{c}_{\mathrm{loc}}(\mathcal{O}_1, b) \geq 1$ *such that*

$$\sup_{0 \leq \tau \leq \bar{\tau}} |\rho(\tau) - \rho^\star|_{l+1}^2 + \sup_{0 \leq \tau \leq \bar{\tau}} |\boldsymbol{v}(\tau) - \boldsymbol{v}^\star|_l^2 + \sup_{0 \leq \tau \leq \bar{\tau}} |T(\tau) - T^\star|_l^2 + \int_0^{\bar{\tau}} |\boldsymbol{v}(\tau) - \boldsymbol{v}^\star|_{l+1}^2 d\tau$$

$$+ \int_0^{\bar{\tau}} |T(\tau) - T^\star|_{l+1}^2 d\tau \leq \mathsf{c}_{\mathrm{loc}}^2 \Big(|\rho_0(\tau) - \rho^\star|_{l+1}^2 + |\boldsymbol{v}_0(\tau) - \boldsymbol{v}^\star|_l^2 + |T_0(\tau) - T^\star|_l^2 \Big)$$

Conclusion/Future work

- **Physical aspects**

  Derivation of Cahn-Hilliard equations

  Mixtures with polyatomic species with chemical reactions

  Numerical simulations at the Molecular/Boltzmann/Fluid levels

  Boundary equations at solid walls

- **Mathematical aspects**

  Global existence results around constant equilibrium states

  Global existence results around stationary nonconstant equilibrium states

  Multicomponent mixtures and Cahn-Hilliard equations