Variational and thermodynamically consistent discretization for heat-conducting viscous fluids

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Modelling, PDE analysis and computational mathematics in materials science

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Goal and overview

Navier-Stokes-Fourier equations:

$$\begin{cases} \rho(\partial_t u + u\cdot\nabla u) = -\nabla p - \rho\nabla\phi + \operatorname{div}\sigma, & p = \dfrac{\partial\epsilon}{\partial\rho}\rho + \dfrac{\partial\epsilon}{\partial s}s - \epsilon \\ \partial_t\rho + \operatorname{div}(\rho u) = 0 & + \text{ boundary conditions!!} \\ T(\partial_t s + \operatorname{div}(su) + \operatorname{div} j) = \sigma : \nabla u - j\cdot\nabla T, & T = \dfrac{\partial\epsilon}{\partial s} \end{cases}$$

Goal I: Geometry (Lie group & variational)
Goal II: Structure preserving + thermodynamically consistent discretization
Red terms: reversible motion (well understood variational/Hamiltonian structure)
Blue terms: irreversible processes:

- thermodynamic fluxes: viscous stress σ, entropy flux j
- thermodynamic forces: ∇u, ∇T

Our approach for (I) and (I): critical action principles

(i) Reversible motion – mechanics:

$$\text{Hamilton principle:} \quad \delta\int_0^T L(q,\dot q)\mathrm{d}t = 0 \; + \text{ arbitrary variations } \delta q$$

(ii) Reversible+irreversible motion – nonequilibrium thermodynamics:

$$\text{d'Alembert type:} \quad \delta\int_0^T L(q,\dot q, S, N, ...)\mathrm{d}t = 0 \; + \text{ variational constraints } \delta q, \delta S, \delta N, \ldots$$

FGB, Yoshimura [2017,2018]

PLAN

1. Variational Thermodynamics:
An extension of Hamilton's principle from mechanics to nonequilibrium thermodynamics

2. Variational formulation for heat conducting viscous fluids

3. Thermodynamically consistent discretization for heat conducting viscous fluids

4. Numerical experiments

1. Variational thermodynamics

1.1 Variational Mechanics: Deduced from Hamilton's principle (first principle)

$$\delta \int_0^T L(q, \dot{q})\mathrm{d}t = 0 \quad \Leftrightarrow \quad \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0$$

– directly related to geometric structures: symplectic and Poisson
– common to a large class of physical theories: Mechanics, Hydrodynamics, Electrodynamics, Relativity, Quantum Mechanics, ...

1.2 Variational Thermodynamics (FGB & Yoshimura [2017]): extension of Hamilton's principle which incorporates irreversible processes (viscosity, heat transfer, diffusion, ...) and entropy evolution

$$\text{Entropy production} \simeq \underbrace{J^\alpha(...)}_{\text{flux}} \cdot \underbrace{X_\alpha}_{\text{force}} \geq 0 \quad \text{De Groot \& Mazur}.$$

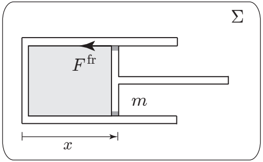
Variational formulation of d'Alembert type. Thermodynamic displacement $\dot{\Lambda}_\alpha = X_\alpha$:

$$\delta \int_0^T L\mathrm{d}t = 0 \;\; \text{s.t.} \begin{cases} \dfrac{\partial L}{\partial S}\dot{\Sigma} = J_\alpha(...) \cdot \dot{\Lambda}^\alpha \; : \text{thermodynamic constraint} \\ \dfrac{\partial L}{\partial S}\delta\Sigma = J_\alpha(...) \cdot \delta\Lambda^\alpha \; : \text{virtual constraint} \end{cases}$$

(later: extension to open systems)

1.3 Finite dimensional examples - isolated systems:

(1) Thermo-mechanical system:



Variational formulation:

$$\delta \int_{t_1}^{t_2} L(q,\dot q,S)\mathrm{d}t = 0 \;\text{ s.t.}\; \begin{cases} \dfrac{\partial L}{\partial S}\dot S = F^{\text{fr}}\cdot \dot q : \text{thermodynamic constraint} \\ \dfrac{\partial L}{\partial S}\delta S = F^{\text{fr}}\cdot \delta q : \text{virtual constraint} \end{cases}$$

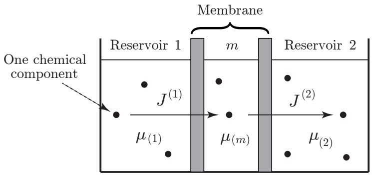
Stationarity conditions:

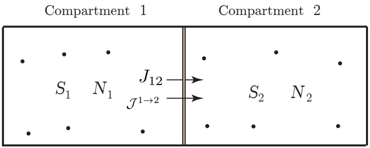
$$\begin{cases} \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot q} - \dfrac{\partial L}{\partial q} = F^{\text{fr}}, \\ \dfrac{\partial L}{\partial S}\dot S = F^{\text{fr}}\cdot \dot q. \end{cases}$$

In this example:

$$J_\alpha \rightsquigarrow F^{\text{fr}} \qquad X^\alpha \rightsquigarrow \dot q \qquad \Lambda^\alpha \rightsquigarrow q$$

(2) Heat and matter transfer:





– Inclusion of diffusion: thermodynamic force X_α:

$$\mu^k = \frac{\partial U}{\partial N_k} : \quad \text{chemical potential of substance in compartment } k$$

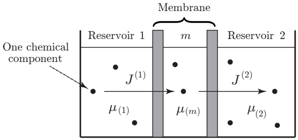
$\rightsquigarrow$ thermodynamic displacements Λ_α: W^k such that $\dot{W}^k = \mu^k$.

– Inclusion of heat conduction: thermodynamic force X_α:

$$T^k = \frac{\partial U}{\partial S_k} : \quad \text{temperature of subsystem } k$$

$\rightsquigarrow$ thermodynamic displacement Λ_α: Γ^k such that $\dot{\Gamma}^k = T^k$
(coincide with the notion of thermal displacement Helmholtz, Green & Naghdi)

Example: systems with friction and diffusion of a single species:



Lagrangian $L = L(q, v, S, N_1, \ldots, N_K)$

Thermodynamic forces/displacements: $v = \dot{q}$ (friction) and $\mu^k = \dot{W}^k$ (diffusion)

Thermodynamic fluxes: $F^{\rm fr}$ (friction) and $\mathcal{J}^{\ell\to k} = -\mathcal{J}^{k\to\ell}$ (diffusion)

$\rightsquigarrow$ our variational principle becomes:

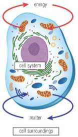
$$\delta \int_{t_1}^{t_2} \left[L(q, \dot{q}, S, N_1, \ldots, N_K) + \dot{W}^k N_k \right] dt = 0 \;\; \text{s.t.} \left\{ \begin{array}{l} \dfrac{\partial L}{\partial S}\dot{S} = \underbrace{F^{\rm fr}\cdot\dot{q}}_{\text{mechanics}} + \displaystyle\sum_{k,\ell} \underbrace{\mathcal{J}^{\ell\to k}\dot{W}^k}_{\text{matter transfer}} \\ \dfrac{\partial L}{\partial S}\delta S = \underbrace{F^{\rm fr}\cdot\delta q}_{\text{virtual}} + \displaystyle\sum_{k,\ell} \underbrace{\mathcal{J}^{\ell\to k}\delta W^k}_{\text{virtual}} \end{array} \right.$$

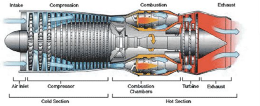
Stationarity conditions:

$$\left\{ \begin{array}{l} \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{q}} - \dfrac{\partial L}{\partial q} = F^{\rm fr}, \qquad \dfrac{d}{dt}N_k = \displaystyle\sum_{\ell=1}^{K} \mathcal{J}^{\ell\to k}, \quad k = 1, \ldots, K, \\ \dfrac{\partial L}{\partial S}\dot{S} = F^{\rm fr}\cdot\dot{q} - \displaystyle\sum_{k<\ell} \mathcal{J}^{\ell\to k}\left(\dfrac{\partial L}{\partial N_k} - \dfrac{\partial L}{\partial N_\ell}\right). \end{array} \right. \quad \& \quad \frac{\partial L}{\partial N_k} = -\dot{W}^k$$

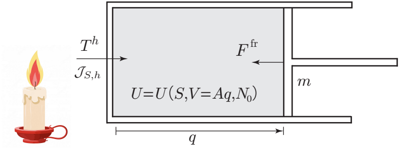
1.4 Finite dimensional examples - open systems:

Open systems:





Thermo-mechanical system with heat source: temperature T^h, entropy flow rate $\mathcal{J}_{S,h}$.



Thermodynamic forces/displacements: $v = \dot{q}$ (friction) and $T = \dot{\Gamma}$ (heating)

Thermodynamic fluxes: F^{fr} (friction) and $\mathcal{J}_{S,h}$ (heating)

New: entropy variable Σ (interpreted later)

$$\delta \int_0^T \left[L(q, \dot{q}, S) + \dot{\Gamma}(S - \Sigma) \right] \mathrm{d}t = 0 \;\; \text{s.t.} \begin{cases} \dfrac{\partial L}{\partial S} \dot{\Sigma} = \underbrace{F^{\mathrm{fr}} \cdot \dot{q}}_{\text{mechanics (int)}} + \underbrace{\mathcal{J}_{S,h}(\dot{\Gamma} - T^h)}_{\text{heat transfer (ext)}} \\ \dfrac{\partial L}{\partial S} \delta \Sigma = \underbrace{F^{\mathrm{fr}} \cdot \delta q}_{\text{virtual}} + \underbrace{\mathcal{J}_{S,h} \delta \Gamma}_{\text{virtual}} \end{cases}$$

Stationarity conditions:

$$\begin{cases} \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot q} - \dfrac{\partial L}{\partial q} = F^{\rm fr}, \qquad \dot S = I + \mathcal{J}_{S,h} \\ I := \dot\Sigma = -\dfrac{1}{T}F^{\rm fr}\dot q + \dfrac{1}{T}\mathcal{J}_{S,h}(T^h - T). \end{cases} \quad \& \quad \frac{\partial L}{\partial S} = -\dot\Gamma$$

Interpretation of Σ:

Prigogine (1917-2003) equations:

$$\mathrm{d}S = \mathrm{d}S_i + \mathrm{d}S_e, \qquad \mathrm{d}S_i \geq 0, \qquad \mathrm{d}S_e \text{ no sign}$$

$\rightsquigarrow$ $\mathrm{d}_i S = \dot\Sigma \mathrm{d}t \geq 0$ and $\mathrm{d}_e S = (\dot S - \dot\Sigma)\mathrm{d}t$ no sign $\quad (\Sigma = \int_{\rm motion}^t \mathrm{d}_i S)$

General form of variational principle for open systems (FGB & Yoshimura [2019]):
α: internal irreversible processes;
β: boundary irreversible processes

$$\delta \int_0^T L\mathrm{d}t = 0 \;\text{ s.t.} \begin{cases} \dfrac{\partial L}{\partial S}\dot\Sigma = J^\alpha \cdot \dot\Lambda_\alpha + J_\beta \cdot (\dot\Lambda^\beta - X^\beta_{\rm ext}) : \text{thermodynamic constraint} \\ \dfrac{\partial L}{\partial S}\delta\Sigma = J^\alpha \cdot \delta\Lambda_\alpha + J_\beta \cdot \delta\Lambda^\beta : \text{virtual constraint} \end{cases}$$

2.1 Lagrangian variational principle: reversible dynamics

– Fluid domain Ω (compact Riemannian manifold with smooth boundary)

– Fluid motion $X \in \Omega \mapsto x = \varphi(t, X) \in \Omega$, with $\varphi(t, \cdot) \in \operatorname{Diff}(\Omega)$

– Lagrangian of a fluid with internal energy $\varepsilon(\rho, s)$:

$$L : T\operatorname{Diff}(\Omega) \to \mathbb{R}, \quad L(\varphi, \dot{\varphi}) = \int_\Omega \Big[\frac{1}{2}\varrho|\dot{\varphi}|^2 - \epsilon\Big(\frac{\varrho}{J\varphi}, \frac{S}{J\varphi}\Big)J\varphi\Big]\mathrm{d}X,$$

$$J\varphi = |\det(\nabla\varphi)| \qquad \varrho(X), S(X) : \text{mass and entropy density.}$$

– Hamilton's principle on the group $\operatorname{Diff}(\Omega)$ of fluid motion

$$\delta\int_0^T L(\varphi, \dot{\varphi})\mathrm{d}t = 0, \ \forall\,\delta\varphi \quad \Longleftrightarrow \quad \varrho\frac{d^2}{dt^2}\varphi = -\nabla p \circ \varphi, \quad p = \rho\frac{\partial\epsilon}{\partial\rho} + s\frac{\partial\epsilon}{\partial s} - \epsilon$$

2.2 Eulerian variational principle: reversible dynamics

- Eulerian fields:

$$u := \dot{\varphi} \circ \varphi^{-1} \qquad \text{Eulerian velocity}$$

$$\rho := (\varrho_0 \circ \varphi^{-1}) J\varphi^{-1} \qquad \text{Eulerian mass density}$$

$$s := (S_0 \circ \varphi^{-1}) J\varphi^{-1} \qquad \text{Eulerian entropy density}$$

- Lagrangian in Eulerian description:

$$\ell(u, \rho, s) = \int_\Omega \left[\frac{1}{2}\rho|u|^2 - \epsilon(\rho, s)\right] \mathrm{d}x$$

- Hamilton's principle in Eulerian form: Euler-Poincaré

$$\delta \int_0^T \ell(u, \rho, s) dt = 0, \quad \delta u = \partial_t \zeta + [u, \zeta], \quad \delta\rho = -\operatorname{div}(\rho\zeta), \quad \delta s = -\operatorname{div}(s\zeta).$$

- Equations of motion:

$$\begin{cases} \partial_t \dfrac{\delta \ell}{\delta u} + \mathcal{L}_u \dfrac{\delta \ell}{\delta u} = \rho \nabla \dfrac{\delta \ell}{\delta \rho} + s \nabla \dfrac{\delta \ell}{\delta s} \\ \partial_t \rho + \operatorname{div}(\rho u) = 0, \quad \partial_t s + \operatorname{div}(su) = 0. \end{cases}$$

Symmetry reduction in Lagrangian mechanics Holm, Marsden, Ratiu [1998].

2.3 Lagrangian variational principle: Viscous heat conducting fluid

FGB, Yoshimura [2018]

Lagrangian: $L : T\,\mathrm{Diff}(\Omega) \times C^\infty(\Omega) \to \mathbb{R}$, $\quad L(\varphi, \dot\varphi, S)$

thermodynamic fluxes: viscosity: viscous stress tensor P

heat conduction: entropy flux J

thermodynamic displacement: viscosity: fluid motion φ $(\dot\varphi = V)$

heat conduction: thermal displacement Γ $(\dot\Gamma = T)$

$+$ entropy variable Σ

Prigogine equations: $\mathrm{d}S = \mathrm{d}_i S + \mathrm{d}_e S$

$\mathrm{d}_i S = \dot\Sigma \mathrm{d}t \geq 0$ & $\mathrm{d}_e S = (\dot S - \dot\Sigma)\mathrm{d}t$ no sign.

VARIATIONAL CONDITION:

$$\delta \int_0^T \left[L(\varphi, \dot\varphi, S)\mathrm{d}t + \int_\Omega \dot\Gamma (S - \Sigma)\mathrm{d}X \right] \mathrm{d}t = 0$$

THERMODYNAMIC CONSTRAINT:

$$\frac{\delta L}{\delta S}\dot\Sigma = -\underbrace{P : \nabla\dot\varphi}_{\text{viscosity}} + \underbrace{J \cdot \nabla\dot\Gamma}_{\text{heat}}$$

VIRTUAL CONSTRAINT:

$$\frac{\delta L}{\delta S}\delta\Sigma = -\underbrace{P : \nabla\delta\varphi}_{\text{virtual}} + \underbrace{J \cdot \nabla\delta\Gamma}_{\text{virtual}}$$

2.4 Eulerian variational description: Viscous heat conducting fluid

Lagrangian $\rightsquigarrow$ Eulerian (reduction by symmetry)

- State variables: $\dot{\varphi}, \varrho, S \rightsquigarrow u, \rho, s$
- Thermodynamic displacements: $\Sigma, \Gamma \rightsquigarrow \varsigma, \gamma$
- Thermodynamic fluxes: $P, J \rightsquigarrow \sigma, j$

Theorem (FGB and Yoshimura [2018])

The variational formulation

$$\delta \int_0^T \left[\ell(u,\rho,s) + \int_\Omega (s-\varsigma) D_t\gamma \mathrm{d}x\right]\mathrm{d}t = 0,$$

with constraints

$$\frac{\delta\ell}{\delta s}\bar{D}_t\varsigma = -\underbrace{\sigma : \nabla u}_{\text{viscosity}} + \underbrace{j\cdot\nabla D_t\gamma}_{\text{heat}}, \qquad \frac{\delta\ell}{\delta s}\bar{D}_\delta\varsigma = -\underbrace{\sigma : \nabla\zeta}_{\text{virtual}} + \underbrace{j\cdot\nabla D_\delta\gamma}_{\text{virtual}}$$

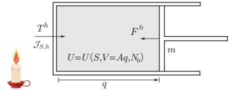
yields the Navier-Stokes-Fourier equations with insulated boundary conditions

$$\begin{cases} \rho(\partial_t u + u\cdot\nabla u) = -\nabla p + \operatorname{div}\sigma, \\ \partial_t\rho + \operatorname{div}(\rho u) = 0 \\ T(\partial_t s + \operatorname{div}(su) + \operatorname{div} j) = \sigma : \nabla u - j\cdot\nabla T \end{cases} \quad \& \quad j\cdot n = 0 \quad \text{on} \quad \partial\Omega$$

2.5 Dirichlet and prescribed flux boundary conditions

$$T = T_0 \quad \text{on} \quad \partial\Omega \qquad \text{or} \qquad Tj \cdot n = q_0 \quad \text{on} \quad \partial\Omega$$

Fluid no more insulated! $\mathrm{d}S = \mathrm{d}_i S + \mathrm{d}_e S$. Recall



$$\delta \int_0^T \left[L(q,\dot q, S) + \dot\Gamma(S-\Sigma)\right]\mathrm{d}t = 0 \;\; \text{s.t.} \begin{cases} \dfrac{\partial L}{\partial S}\dot\Sigma = \underbrace{F^{\rm fr}\cdot \dot q}_{\text{mechanics (int)}} + \underbrace{\mathcal{J}_{S,h}(\dot\Gamma - T^h)}_{\text{heat transfer (ext)}} \\ \dfrac{\partial L}{\partial S}\delta\Sigma = \underbrace{F^{\rm fr}\cdot \delta q}_{\text{virtual}} + \underbrace{\mathcal{J}_{S,h}\delta\Gamma}_{\text{virtual}} \end{cases}$$

(A) Dirichlet boundary conditions:

$$\int_\Omega W \frac{\delta L}{\delta S}\dot\Sigma \,\mathrm{d}X = -\int_\Omega W \underbrace{(P : \nabla\dot\varphi)}_{\text{viscosity}}\mathrm{d}X + \int_\Omega W \underbrace{(J_S \cdot \nabla\dot\Gamma)}_{\text{heat conduction}}\mathrm{d}X - \int_{\partial\Omega} W \underbrace{(J_S\cdot n)(\dot\Gamma - \mathfrak{T}_0)}_{\text{heat transfer}}\mathrm{d}A, \forall W$$

$$\int_\Omega W \frac{\delta L}{\delta S}\delta\Sigma \,\mathrm{d}X = -\int_\Omega W \underbrace{(P : \nabla\delta\varphi)}_{\text{viscosity}}\mathrm{d}X + \int_\Omega W \underbrace{(J_S \cdot \nabla\delta\Gamma)}_{\text{heat conduction}}\mathrm{d}X - \int_{\partial\Omega} W \underbrace{(J_S\cdot n)\delta\Gamma}_{\text{heat transfer}}\mathrm{d}A, \forall W,$$

(B) Prescribed flux boundary conditions:

$$\int_{\partial\Omega} W \underbrace{(J_S\cdot n)(\dot\Gamma - \mathfrak{T}_0)}_{\text{heat transfer}}\mathrm{d}A \;\rightsquigarrow\; \int_{\partial\Omega} W \underbrace{((J_S\cdot n)\dot\Gamma - \mathfrak{Q}_0)}_{\text{heat transfer}}\mathrm{d}A, \forall W$$

Theorem (Gawlik and FGB [2023])

The variational formulation

$$\delta \int_0^T \left[\ell(u,\rho,s) + \int_\Omega (s-\varsigma) D_t\gamma \mathrm{d}x\right] \mathrm{d}t = 0,$$

with constraints

$$\int_\Omega w \frac{\delta \ell}{\delta s} \bar{D}_t \varsigma \,\mathrm{d}x = -\int_\Omega w \underbrace{(\sigma : \nabla u)}_{\text{viscosity}} \mathrm{d}x + \int_\Omega w \underbrace{(j \cdot \nabla D_t\gamma)}_{\text{heat}} \mathrm{d}x - \int_{\partial\Omega} w \underbrace{(j\cdot n)(D_t\gamma - T_0)}_{\text{heat transfer}} \mathrm{d}a, \forall w$$

$$\int_\Omega w \frac{\delta \ell}{\delta s} \bar{D}_\delta \varsigma \,\mathrm{d}x = -\int_\Omega w \underbrace{(\sigma : \nabla \zeta)}_{\text{virtual}} \mathrm{d}x + \int_\Omega w \underbrace{(j \cdot \nabla D_\delta\gamma)}_{\text{virtual}} \mathrm{d}x - \int_{\partial\Omega} w \underbrace{(j\cdot n) D_\delta\gamma}_{\text{virtual}} \mathrm{d}a, \forall w.$$

yields the Navier-Stokes-Fourier equations with Dirichlet boundary conditions

$$\begin{cases} \rho(\partial_t u + u\cdot\nabla u) = -\nabla p + \operatorname{div}\sigma, \\ \partial_t \rho + \operatorname{div}(\rho u) = 0 \\ T(\partial_t s + \operatorname{div}(su) + \operatorname{div} j) = \sigma : \nabla u - j\cdot\nabla T \end{cases} \quad \& \quad T = T_0 \quad \text{on} \quad \partial\Omega$$

Similarly for prescribed heat flux.

$$\rightsquigarrow \frac{d}{dt}\mathcal{E} = -\int_{\partial\Omega} (j\cdot n) T_0 \,\mathrm{d}a.$$

Interlude: Geometric description of the constraints

Kinematic (C_K) and variational (C_V) constraint submanifolds.

(1) Nonholonomic mechanics with linear constraints: $\Delta \subset T\mathcal{Q}$ distribution
Locally:

$$A^\ell_i(x)\dot{x}^i = 0 \longleftrightarrow A^\ell_i(x)\delta x^i = 0, \quad \ell = 1, ..., N$$

(2) Thermodynamics of isolated systems: $C_V \subset T\mathcal{Q} \times_{\mathcal{Q}} T\mathcal{Q} \leftrightarrow C_K \subset T\mathcal{Q}$
Locally:

$$A^\ell_i(x, \dot{x})\dot{x}^i = 0 \longleftrightarrow A^\ell_i(x, \dot{x})\delta x^i = 0, \quad \ell = 1, ..., N$$

This relation $C_V \leftrightarrow C_K$ allows a formulation with Dirac structures.

(3) Open thermodynamics: $C_V \subset (\mathbb{R} \times T\mathcal{Q}) \times_{\mathbb{R}\times\mathcal{Q}} T(\mathbb{R} \times \mathcal{Q}) \leftrightarrow C_K \subset T(\mathbb{R} \times \mathcal{Q})$ Locally:

$$A^\ell_i(t, x, \dot{x})\dot{x}^i + B^\ell(t, x, \dot{x})\dot{t} = 0 \longleftrightarrow A^\ell_i(t, x, \dot{x})\delta x^i + B^\ell(t, x, \dot{x})\underbrace{\delta t}_{=0} = 0, \quad \ell = 1, ..., N$$

Appropriate geometric setting: bundle $\mathcal{Y} = \mathbb{R} \times \mathcal{Q} \to \mathbb{R}$
Lagrangian defined on $J^1\mathcal{Y} = \mathbb{R} \times T\mathcal{Q}$ Gotay et al. [1997]; Giachetta et al. [1997]

Variational constraint: $C_V \subset J^1\mathcal{Y} \times_{\mathcal{Y}} T\mathcal{Y}$.
Relation $C_V \leftrightarrow C_K$ allows a formulation with Dirac structures.

Both Dirac structure formulation and bracket formulations (metriplectic, double & single generator) can be derived from the variational setting (Eldred & FGB)

3. Thermodynamically consistent & variational discretization for heat conducting viscous fluids

3.1 Discrete Lie group formulation

- "replace" Diff(Ω) by a finite dimensional Lie group approximation
- apply the variational principles on this finite dimensional Lie group
- temporal discretization in a structure preserving way

Original idea: Pavlov, Mullen, Tong, Kanso, Marsden, Desbrun [2010]

3.2 Geometric variational finite elements for compressible fluids

- STEP 1: Define the discrete diffeomorphism group $\sim GL(V_h)$
- STEP 2: Relate the Lie algebra $\sim \mathfrak{gl}(V_h)$ of this group with discrete velocities $(u \in H_0(\mathrm{div}, \Omega) \to A_u \in \mathfrak{gl}(V_h))$.
- STEP 3: Show that the subspace of discrete velocities is a Raviart-Thomas space $V_h = DG_r(\mathcal{T}_h) \Rightarrow RT_{2r}(\mathcal{T}_h)$ (Gawlik, FGB [2020])
- STEP 4: Reversible case: apply the variational formulation (Hamilton's principle) on the discrete diffeomorphism group
  $\Rightarrow$ FINITE ELEMENT SCHEME (& choice of finite element space for u)

STEP 1: Discrete diffeomorphism groups

- Discrete functions: finite element space $V_h \subset L^2(\Omega)$ associated to $\mathcal{T}_h$ (shape-regular and quasi-uniform family $\{\mathcal{T}_h\}$)

- Finite dimensional version of $\mathrm{Diff}(\Omega)$: chosen as

$$G_h = \{g \in GL(V_h) \mid g \cdot \mathbf{1} = \mathbf{1}\},$$

$v \in V_h \mapsto g \cdot v \in V_h$ discrete version of $f \in \mathcal{F} \mapsto \varphi \cdot f := f \circ \varphi^{-1} \in \mathcal{F}$.

- Lie algebra

$$\mathfrak{g}_h = \{A \in L(V_h, V_h) \mid A \cdot \mathbf{1} = 0\}$$

Discrete version of the Lie algebra of $\mathrm{Diff}(\Omega)$:

$v \in V_h \mapsto A \cdot v \in V_h$ discrete version of $f \in \mathcal{F} \mapsto u \cdot f := -u \cdot \nabla f \in \mathcal{F}$.

$\rightsquigarrow$ Potential candidates to be discrete vector fields;
$\rightsquigarrow$ As linear maps these discrete vector fields act as discrete derivations on V_h;
$\rightsquigarrow$ Natural to choose them as discrete distributional directional derivatives.

STEP 2: Link with discrete velocities

$H_0(\mathrm{div},\Omega) = \{u \in H(\mathrm{div},\Omega) \mid u \cdot n = 0 \text{ on } \partial\Omega\}$, $V_h = V_h^r$.

Theorem (Gawlik and FGB)

- To each velocity $u \in H_0(\mathrm{div},\Omega) \cap L^p(\Omega)^n$, $p > 2$, $r \geq 0$ integer, we can associate the Lie algebra element $A_u \in \mathfrak{gl}(V_h^r)$ given by

$$\langle A_u f, g\rangle := \sum_{K\in\mathcal{T}_h} \int_K (\nabla_u f) g \,\mathrm{d}x - \sum_{e\in\mathcal{E}_h^0} \int_e u \cdot [\![f]\!]\{g\}\,\mathrm{d}s, \quad \forall\, f,g \in V_h^r.$$

- A_u is consistent approximation of the distributional derivative in direction u.

STEP 3: Relation with Raviart-Thomas finite element spaces

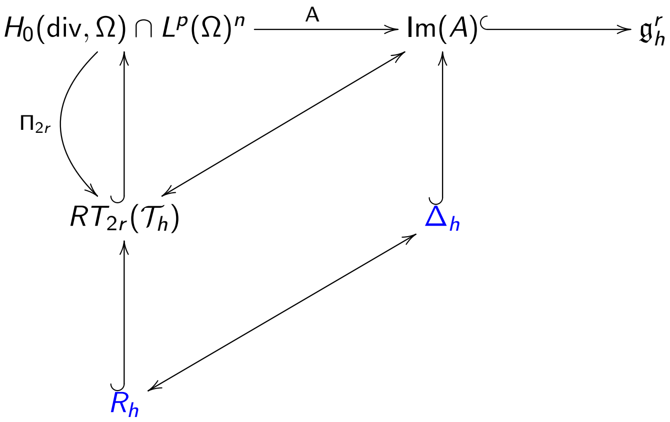
Theorem (Gawlik and FGB)

The space $\{A_u \mid u \in H_0(\mathrm{div},\Omega) \cap L^p(\Omega)^n, p > 2\}$ is isomorphic to the Raviart-Thomas space of order $2r$

$$RT_{2r}(\mathcal{T}_h) = \left\{u \in H_0(\mathrm{div},\Omega) \mid u|_K \in (P_{2r}(K))^n + xP_{2r}(K),\, \forall K \in \mathcal{T}_h\right\}.$$

Link between the geometric variational discretization and finite element methods.

SUMMARY OF GEOMETRIC VARIATIONAL SETTING



Choice of final finite element space Δ_h:
such that the discrete Lagrangian is hyperregular.

Example: barotropic fluid
$\rho \in V_h = DG_r(\mathcal{T}_h)$;
$u \in \Delta_h = BDM_r(\mathcal{T}_h) \subset RT_{2r}(\mathcal{T}_h) \subset \mathfrak{gl}(V_h)$:

- Equations of motion (Euler-Poincaré form, $A \in \mathfrak{gl}(V_h)$)

$$\delta \int_0^T \ell(A,\rho)\mathrm{d}t = 0 \Rightarrow \begin{cases} \left\langle \partial_t(\rho A), B \right\rangle + \left\langle \rho A, [A,B] \right\rangle + \left\langle \pi_h\left(\frac{1}{2}|A|^2 - e(\rho) - \rho\frac{\partial e}{\partial \rho}\right), \rho \cdot B \right\rangle = 0, \\ \left\langle \partial_t \rho, \sigma \right\rangle + \left\langle \rho, A\sigma \right\rangle = 0, \quad \forall \sigma \in DG_r(\mathcal{T}_h), \quad \forall B \in BDM_r(\mathcal{T}_h). \end{cases}$$

- Equivalently (finite element form, $u \in BDM_r(\mathcal{T}_h)$):

$$\begin{cases} \left\langle \partial_t(\rho u), v \right\rangle + a_h(\rho u, u, v) - b_h(v, f, \rho) = 0, \quad \forall v \in BDM_r(\mathcal{T}_h) \\ \left\langle \partial_t \rho, \sigma \right\rangle - b_h(u, \sigma, \rho) = 0, \quad \forall \sigma \in DG_r(\mathcal{T}_h), \end{cases}$$

- $f = \pi_h\left(\frac{1}{2}|u|^2 - e(\rho) - \rho\frac{\partial e}{\partial \rho}\right)$
- $a_h(w,u,v) = \sum_{K \in \mathcal{T}_h} \int_K w \cdot (v \cdot \nabla u - u \cdot \nabla v)\, \mathrm{d}x + \sum_{e \in \mathcal{E}_h^0} \int_e (v \cdot n[u] - u \cdot n[v]) \cdot \{w\} \mathrm{d}s$
- $b_h(w,f,g) = \sum_{K \in \mathcal{T}_h} \int_K (w \cdot \nabla f) g \, \mathrm{d}x - \sum_{e \in \mathcal{E}_h^0} w \cdot [[f]]\{g\}\mathrm{d}s.$

3.3 Temporal discretization

OPTION 1: variational discretization

OPTION 2: energy preserving discretization

$$\begin{cases} \left\langle \frac{\rho_{k+1}u_{k+1}-\rho_k u_k}{\Delta t}, v\right\rangle + a_h\left(\frac{\rho_k u_k+\rho_{k+1}u_{k+1}}{2}, \frac{u_k+u_{k+1}}{2}, v\right) \\ \qquad -b_h\left(v, \pi_h\left(\frac{1}{2}u_k\cdot u_{k+1} - f(\rho_k,\rho_{k+1})\right), \frac{\rho_k+\rho_{k+1}}{2}\right) = 0, \quad \forall v \in BDM_r(\mathcal{T}_h) \\ \left\langle \frac{\rho_{k+1}-\rho_k}{\Delta t}, \sigma\right\rangle - b_h\left(\frac{u_k+u_{k+1}}{2}, \sigma, \frac{\rho_k+\rho_{k+1}}{2}\right) = 0, \quad \forall \sigma \in DG_r(\mathcal{T}_h), \end{cases}$$

where $f(x,y) = \frac{ye(y)-xe(x)}{y-x}$ (reminiscent of a discrete gradient method Hairer, Lubich, Wanner [2006])

Convergence (for $R_h = RT_r(\mathcal{T}_h)$):
- h: optimal (order $r+1$) when $r=0$; suboptimal when $r>0$, but still grows with r.
- Δt: second order.

Exact preservation of $\int_\Omega \left[\frac{1}{2}\rho_k|u_k|^2 + \varepsilon(\rho_k)\right]\mathrm{d}x$ & $\int_\Omega \rho_k \mathrm{d}x$
(& div $u_k = 0$ & $\int_\Omega \rho_k^2 \mathrm{d}x$ for incomp. with variable density.)
(& div $B_k = 0$ & magnetic Helicity for MHD)
(& cross-Helicity for incomp. MHD)

3.4 Variational finite element scheme for heat conducting viscous fluids

As before:

- "replace" $\mathrm{Diff}(\Omega)$ by a finite dimensional Lie group approximation
- apply variational thermodynamics on this finite dimensional Lie group
- temporal discretization in a structure preserving way

No-slip boundary conditions for u:

$$CG_r(\mathcal{T}_h)^n := \{u \in H^1_0(\Omega)^n \mid u|_K \in P_r(K)^n,\ \forall\, K \in \mathcal{T}_h\} \subset \mathfrak{gl}(V_h)$$

Main step: discretization of the fluxes σ and j. Focus on Navier-Stokes-Fourier fluid:

Navier-Stokes : $\sigma = \sigma(u) = 2\mu\,\mathrm{Def}\,u + \lambda(\mathrm{div}\,u)\delta,\qquad \mu \geq 0,\ \zeta = \lambda + \frac{2}{3}\mu \geq 0$

Fourier's law : $j_s = j_s(T) = -\frac{1}{T}\kappa\nabla T,\qquad \kappa \geq 0.$

$$\text{viscosity}: \quad c(w,u,v) = \int_\Omega w\,\sigma(u) : \nabla v\,\mathrm{d}x.$$

$$\text{heat conduction}: \quad d(w,f,g) = \int_\Omega w\,j_s(f)\cdot\nabla g\,\mathrm{d}x$$

$\rightsquigarrow$ $c_h : L^\infty(\Omega) \times H^1_0(\Omega)^n \times H^1_0(\Omega)^n \to \mathbb{R}$ trilinear

$\rightsquigarrow$ $d_h : V_h \times V_h \times V_h \to \mathbb{R}$ linear in first and last argument

Theorem I: discrete variational formulation (Gawlik and FGB [2023])

The variational formulation

$$\delta \int_0^T \left[\ell_d(A,\rho,s) + \langle s - \varsigma, D_t^h \gamma \rangle\right] \mathrm{d}t = 0,$$

with constraints

$$\left\langle \frac{\partial \ell_d}{\partial s} D_t^h \varsigma, w \right\rangle = -c_h(w, A, A) + d_h\left(w, -\frac{\partial \ell_d}{\partial s}, D_t^h \gamma\right), \quad \forall w \in DG_r(\mathcal{T}_h),$$

$$\left\langle \frac{\partial \ell_d}{\partial s} D_\delta^h \varsigma, w \right\rangle = -c_h(w, A, B) + d_h\left(w, -\frac{\partial \ell_d}{\partial s}, D_\delta^h \gamma\right), \quad \forall w \in DG_r(\mathcal{T}_h),$$

yields the following finite element discretization of the Navier-Stokes-Fourier equations

Find $u \in CG_r(\mathcal{T}_h)$, $\rho, s \in DG_r(\mathcal{T}_h)$ such that

$$\begin{cases} \langle \partial_t(\rho u), v\rangle + a_h(\rho u, u, v) - b_h(v, f, \rho) + b_h(v, T, s) = -c_h(1, u, v), \ \forall\, v \in CG_r(\mathcal{T}_h), \\ \langle \partial_t \rho, \sigma\rangle - b_h(u, \sigma, \rho) = 0, \ \forall\, \sigma \in DG_r(\mathcal{T}_h), \\ \langle \partial_t s, Tw\rangle - b_h(u, Tw, s) - d_h(1, T, Tw) = c_h(w, u, u) - d_h(w, T, T), \ \forall\, w \in DG_r(\mathcal{T}_h), \end{cases}$$

$$T := -\frac{\partial \ell_d}{\partial s} = \pi_h \frac{\delta \ell}{\delta S}$$

Choose:

$$
\begin{aligned}
c_h(w,u,v) &= c(w,u,v)\\
d_h(w,f,g) &= -\kappa \sum_{K\in\mathcal{T}_h}\int_K \frac{w}{f}\nabla f\cdot\nabla g\,\mathrm{d}x + \kappa\sum_{e\in\mathcal{E}_h^0}\int_e \frac{1}{\{f\}}\{w\nabla f\}\cdot[[g]]\,\mathrm{d}a\\
&\quad -\kappa\sum_{e\in\mathcal{E}_h^0}\int_e\frac{1}{\{f\}}\{w\nabla g\}\cdot[[f]]\,\mathrm{d}a - \sum_{e\in\mathcal{E}_h^0}\frac{\eta}{h_e}\int_e\frac{\{w\}}{\{f\}}[[f]]\cdot[[g]]\,\mathrm{d}a,
\end{aligned}
$$

d_h: standard non-symmetric interior penalty discretization (for problems with Neuman b.c.) (Brenner and Scott [2008]) boundedness and coercive properties.

Crucial step: $\Rightarrow$ CAN be followed by a thermodynamically consistent temporal discretization!

$$
\begin{cases}
\left\langle \dfrac{\rho_{k+1} u_{k+1} - \rho_k u_k}{\Delta t}, v \right\rangle + a_h\Big(\dfrac{\rho_k u_k + \rho_{k+1} u_{k+1}}{2}, \dfrac{u_k + u_{k+1}}{2}, v \Big) \\
\quad - b_h\Big(v, \pi_h\big(\tfrac{1}{2} u_k \cdot u_{k+1}\big) - D_1\epsilon, \dfrac{\rho_k + \rho_{k+1}}{2} \Big) + b_h\big(v, D_2\epsilon, \dfrac{s_k + s_{k+1}}{2}\big) = -c\big(1, \dfrac{u_k + u_{k+1}}{2}, v\big) \\
\left\langle \dfrac{\rho_{k+1} - \rho_k}{\Delta t}, \sigma \right\rangle - b_h\Big(\dfrac{u_k + u_{k+1}}{2}, \sigma, \dfrac{\rho_k + \rho_{k+1}}{2} \Big) = 0, \\
\left\langle \dfrac{s_{k+1} - s_k}{\Delta t}, D_2\epsilon w \right\rangle - b_h\Big(\dfrac{u_k + u_{k+1}}{2}, D_2\epsilon w, \dfrac{s_k + s_{k+1}}{2} \Big) \\
\quad - d_h(1, D_2\epsilon, D_2\epsilon w) = c\big(w, \dfrac{u_k + u_{k+1}}{2}, \dfrac{u_k + u_{k+1}}{2}\big) - d_h(w, D_2\epsilon, D_2\epsilon),
\end{cases}
$$

for all $v \in CG_r(\mathcal{T}_h)^n$ and all $\sigma, w \in DG_r(\mathcal{T}_h)$.

$$
D_1\epsilon = \pi_h \left(\frac{\delta_1(\rho_k, \rho_{k+1}, s_k) + \delta_1(\rho_k, \rho_{k+1}, s_{k+1})}{2} \right), \qquad \delta_1(\rho, \rho', s) = \frac{\epsilon(\rho', s) - \epsilon(\rho, s)}{\rho' - \rho}
$$

$$
D_2\epsilon = \pi_h \left(\frac{\delta_2(s_k, s_{k+1}, \rho_k) + \delta_2(s_k, s_{k+1}, \rho_{k+1})}{2} \right), \qquad \delta_2(s, s', \rho) = \frac{\epsilon(\rho, s') - \epsilon(\rho, s)}{s' - s}
$$

still reminiscent of a discrete gradient method, but followed by a midpoint rule for the other variable

Theorem II: fully discrete thermodynamic consistency (Gawlik and FGB [2022])

The fully discrete solution of the Navier-Stokes-Fourier equation satisfies

$$\int_\Omega \rho_{k+1} \mathrm{d}x = \int_\Omega \rho_k \mathrm{d}x \quad \text{mass conservation}$$

$$\int_\Omega \left[\frac{1}{2}\rho_{k+1}|u_{k+1}|^2 + \epsilon(\rho_{k+1}, s_{k+1}) \right] \mathrm{d}x = \int_\Omega \left[\frac{1}{2}\rho_k |u_k|^2 + \epsilon(\rho_k, s_k) \right] \mathrm{d}x \quad 1^{st} \text{ law}$$

$$\left\langle \frac{s_{k+1} - s_k}{\Delta t}, T_{[k]} w \right\rangle + b\left(T_{[k]} w, s_{k+1/2}, u_{k+1/2}\right) + d\left(1, T_{[k]}, T_{[k]} w\right) \geq 0, \ \forall w \geq 0, \quad 2^{nd} \text{ law}$$

Discrete temperature $T_{[k]}$: mean value in ρ of discrete gradient $\frac{\epsilon(\rho, s_{k+1}) - \epsilon(\rho, s_k)}{s_{k+1} - s_k}$.

Previous works only achieve some of these properties (for some boundary conditions):
Hughes, Franca, Mallet [1986] and Shakib, Hughes, Johan [1991]: global entropy production, no balance of total energy.
Tadmor, Zhong [2006] global entropy production in the one-dimensional setting.
Basarić, Lukáčová-Medviďová, Mizerová, She, Yuan. [2023]: global energy conservation, global (not local) entropy production, artificial source of energy dissipation and entropy production.

3.5 Enhancements

1) Prescribed temperature and prescribed heat flux B.C. (hard):

So far insulated B.C.: $j \cdot n|_{\partial\Omega} = 0$

Now $T|_{\partial\Omega} = T_0$ or $Tj \cdot n|_{\partial\Omega} = q_0$

$\rightsquigarrow$ use the variational formulation for open systems

$\rightsquigarrow$ changes in d_h and e_h

$\rightsquigarrow$ theorem II satisfied (first and second law for open systems)

2) Rotation and gravity (easy):

$\rightsquigarrow$ in the Lagrangian: theorem II satisfied

3) Variable coefficients (easy):

viscosity $\mu(\rho, T)$ and $\zeta(\rho, T)$

$\rightsquigarrow$ $c(w, \frac{u_k+u_{k+1}}{2}, \frac{u_k+u_{k+1}}{2})$ evaluated at $(\rho, T) = (\rho_{k+1/2}, D_2\epsilon)$: theorem II satisfied

heat conduction $\kappa(\rho, T)$

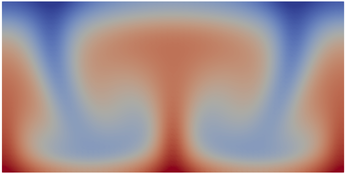
$\rightsquigarrow$ careful with the trace of $\kappa(\rho, f)$ (such as $\{\kappa(\rho, f)\}$ or $\kappa(\{\rho\}, \{f\})$) when treating integrals over $e \in \mathcal{E}_h^0$: theorem II satisfied

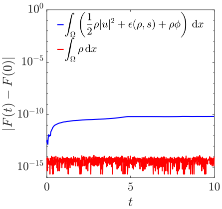
4) Upwinding (easy):

$\rightsquigarrow$ $b \to \tilde{b}$ everywhere (Gawlik&FGB [2020]): theorem II satisfied.

3.6 Rayleigh-Bénard convection

- Convection driven by a temperature difference between the top and bottom boundaries
- Ubiquitous in nature: occurring in oceans, atmospheres and mantles of planets, in stars
- Equilibrium state $T(x, y, z) = T_0 + Z(1 - z)$, $u(x, y, z) = 0$. Stability? Onset of convection?
- Most of analytical and numerical studies: Boussinesq approximation (valid only for thin layers, no thermodynamics) Stable $\Leftrightarrow$ $\mathrm{Ra} < \mathrm{Ra}_c \sim 1708$ (Ra=Rayleigh number)
- Complete model: onset of convection much more difficult to analyse (Ra_c not fixed) Bormann [2001], Alboussière, Ricard [2017].





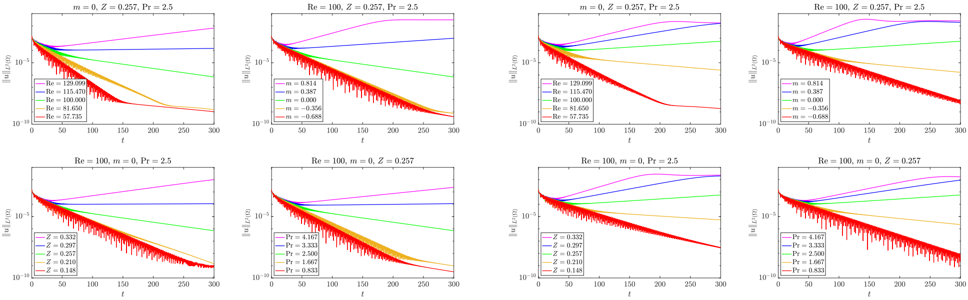
$\mathrm{Ra} := \mathrm{Re}^2(m + 1)Z^2\mathrm{Pr}(1 - (\gamma - 1)m)/\gamma$

Left: $\mathrm{Re} = 100$, $m = 0$, $Z = 2$, $\mathrm{Pr} = 2.5$, so $\mathrm{Ra} = 90909.1$. $\gamma = 1.1$ ($h = 0.03125$, at $t = 14.5$).

Right: Evolution of mass and energy during the simulation. The absolute deviations $|F(t) - F(0)|$ are plotted for each conserved quantity $F(t)$.

- Boundary conditions matter:

Dirichlet boundary conditions VS Prescribed heat flux:



Start with: $\mathrm{Re} = 100$, $m = 0$, $Z = 0.256905$, $\mathrm{Pr} = 2.5$, so $\mathrm{Ra} = 1500$.
Vary each parameter to that $\mathrm{Ra} \in \{500, 1000, 1500, 2000, 2500\}$.
$h = \frac{\sqrt{2}}{16}$, $\Delta t = 0.4$, $\eta = 0.01$, $V_h = DG_1(\mathcal{T}_h)$, $u \in CG_2(\mathcal{T}_h)^2$.

Change of boundary conditions "prescribed temperature $\rightarrow$ prescribed flux" has a significant impact on the onset of convection by decreasing the critical Rayleigh number $\mathrm{Ra}_c \in [1500, 2000] \rightarrow \mathrm{Ra}_c \in [1000, 1500]$ (green-blue $\rightarrow$ yellow-green) (for Boussinesq Hurle, Jakeman, Pike [1967], Chapman, Proctor [1980]).

4. Conclusion

- Show the geometric Lie group variational formulation for heat conducting viscous fluids. Consistent extension of the geometric Lie group variational formulation of Euler equations.

- Used the framework of Variational Thermodynamics (modified Hamilton's principle – d'Alembert type
$$\delta \int L\mathrm{d}t = 0 + (\text{flux} \times \text{forces}) \text{ constraints})$$
- Applied it to a discrete version of diffeomorphism group
- Derived a thermodynamic consistent finite element for Navier-Stokes-Fourier (two laws at the fully discrete level). The first such scheme, a.f.a.w.n.
- Form of entropy equation resulting from the variational approach plays a main role
- Insulated, Dirichlet, and prescribed flux boundary conditions can be treated by using appropriate variational formulation.
- Besides numerics: variational formulation provides a unified perspective for geometric formulations and modelling in thermodynamics:
  $\rightsquigarrow$ derive bracket formulations (single and double generators) Eldred & FGB [2020]
  $\rightsquigarrow$ derive Dirac structure formulations FGB & Yoshimura [2020]
  $\rightsquigarrow$ thermodynamically consistent modelling in geophysical fluids, porous media, ...

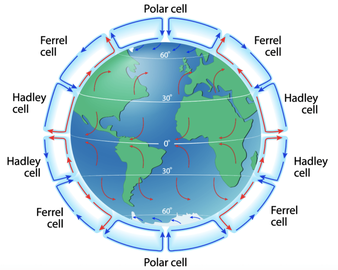
Variational discretization:
– Gawlik, E.S. and FGB [2020], A variational finite element discretization of compressible flow. Found. Comput. Math. 21, 961–1001 (2020)
– Gawlik, E.S. and FGB [2023], Variational and thermodynamically consistent finite element discretization for heat conducting viscous fluids. *Mathematical Models and Methods in Applied Sciences*

Overview of our variational formulation:
FGB and H. Yoshimura [2019], From Lagrangian mechanics to nonequilibrium thermodynamics: a variational perspective, *Entropy*, 21(1), 8

Modelling:
– FGB [2019], A variational derivation of the nonequilibrium thermodynamics of a moist atmosphere with rain process and its pseudoincompressible approximation, Geophysical & Astrophysical Fluid Dynamics, 113:5-6, 428–465.
– Eldred, C. and FGB [2021], Thermodynamically consistent semi-compressible fluids: a variational perspective, J. Phys. A, 54, 345701.
– FGB and V. Putkaradze [2022], Variational geometric approach to the thermodynamics of porous media, ZAMM, 102(11).

From variational to bracket formulations:
– FGB and H. Yoshimura [2020], From variational to bracket formulations in nonequilibrium thermodynamics of simple systems, J. Geom. Phys., 158, 103812.
– Eldred, C. and FGB [2020], Single and double generator bracket formulations of multicomponent fluids with irreversible processes, J. Phys. A, 53(39), 395701.

From variational formulation to Dirac structures:
– FGB and H. Yoshimura [2018], Dirac structures in nonequilibrium thermodynamics, J. Math. Phys., 59, 012701.
– FGB and H. Yoshimura [2020], Dirac structures in nonequilibrium thermodynamics for simple



THANK YOU

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