Phase stability for mixed fluids by Global Optimization using symplectic trajectories

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DFG-Research Center MATHEON
Mathematics for Key Technologies.

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Outline

1. Phase Equilibium ⇒ Seminfinite programme
   ⇓ (Duality)
2. Tangent Plane Criterion ⇒ Global Optimization
   ⇓ (Search Heuristic)
3. Hamiltonian system of ODEs
   ⇓ (Discretization)
4. Mid-point rule ⇒ Sequence of NLPs
   ⇓ (quasi-Newton method)
5. Linear Algebra of shifted/updated Hessian

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Problem description

- Mixed Fluid (e.g. Reservior Oil)
- Controlled Temperature and Pressure
- Feed $m = (m_1, m_2, \dots, m_n) > 0$, $m_i \equiv$ moles of species i.
- Norm: $b(m) \equiv$ hard sphere volume
  $\leqslant$ volume v occupied by m.
- Molar density $d \equiv m/v \in \mathcal{D} = \{0 \leqslant d \in \mathbb{R}^n : b(d) \leqslant 1\}$.
- Energy density $E(d) \equiv \frac{1}{v} G(m, v) = G(d, 1)$ (Gibb's Free Energy).
- Assumptions $E : \mathcal{D} \longrightarrow \mathbb{R} \cup \{\infty\}$
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  $\frac{\partial E}{\partial n} = \infty$ on boundary.

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Primal and Dual problems

Primal Problem With $d_i \in \mathcal{D}\,, v_i \in \mathbb{R}$ for $i = 1, \ldots, p \geqslant 1$

$$\min \sum_{i=1}^{p} v_i E(d_i) \quad \text{s. t.} \quad \sum_{i=1}^{p} v_i d_i = m\,.$$

$$\Updownarrow$$

Dual Problem For $g \in (\mathbb{R}^n)^p$

$$\max g^\top m \quad \text{s. t.} \quad g^\top d \leqslant E(d)\ \forall d \in \mathcal{D}$$

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Duality principles

Weak Duality For every feasible point $(d_i, v_i)_{i=1}^p$ and g satisfying $g^\top d \leqslant E(d)\ \forall d \in \mathcal{D}$ we have

$$\sum_{i=1}^{p} v_i E(d_i) \geqslant \sum_{i=1}^{p} v_i g^\top d_i = g^\top \sum_{i=1}^{p} v_i d_i = g^\top m\,.$$

Strong Duality For every $m > 0\ \exists d_i^* \in \mathcal{D}$ and $v_i^* > 0$ $\forall i = 1, \ldots, p$ as well as $g_* \in \mathbb{R}^n$ such that

$$G_*(m) \equiv \sum_{i=1}^{p} v_i^* E(d_i^*) = g_*^\top m \text{ with } p \leqslant n\,.$$

where G_* is the convex conic hull of E.

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Tangent plane criterion

For each p solving the optimization problem locally gives us points $d_i^* \in \mathcal{D}$ and a Lagrange multiplier vector $g_* = \nabla E(d_i^*)\ \forall i = 1, \ldots, p$, which satisfy the KKT conditions. This point is globally stable if and only if

$$t(d) = E(d) - g_*^\top d \geqslant 0\ \forall d \in \mathcal{D}$$

and

$$t(d_i^*) = 0\ \forall i = 1, \ldots, p\,.$$

Here $t(d)$ forms a tangent plane to the energy surface at the points d_i^*. The question is whether or not does the energy surface intersect the tangent plane, so that $t(d) < 0$ at such a point $d \in \mathcal{D}$.

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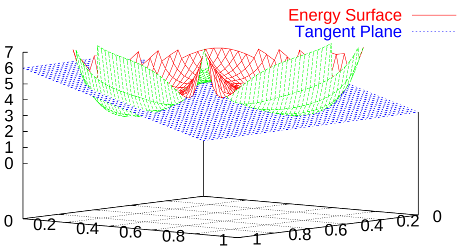
Tangent plane criterion

Instable One Phase



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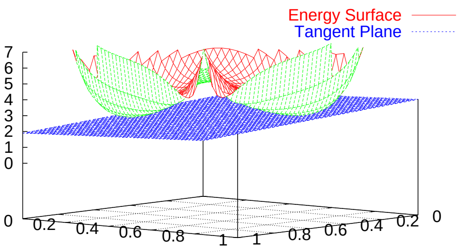

we need to find the whether the global minimum of $t(d)$ is less than 0, in which case, this phase split is unstable and we obtain a split into $p + 1$ phases. $t(d)$ is, essentially, a smooth but non convex objective on the compact domain $\mathcal{D} \subset \mathbb{R}^n$.

Global Optimization – Observations

i. Mostly “optimization” $\equiv$ local optimization.
ii. Local $\Rightarrow$ global only for “convex” case.
iii. Rigorous global optimization
    - space covering (requires Lipschitz constants)
    - curse of dimensionality
iv. Stochastic optimization
    - convergence with probability 1
    - no reliable stoping criteria
v. Averaging seems to be a good idea if the function can be considered as a sum of an overall convex function and a bounded purturbation.

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Hamiltonian trajectory search

Suppose $f(x)\ \nabla f(x)$ known on trajectory $x(\tau)$, $0 \leqslant \tau \leqslant t$.

Question Which direction $\dot{x}(t)$ to move in?

Answer $\dot{x}(t) = \dot{x}(0) + \int_0^t -[\nabla f(x(\tau))\sigma(f(x(\tau)))]\mathrm{d}\tau$

$$\iff \ddot{x}(t) = -\sigma(f(x(t)))\nabla f(x(t))$$

Sensitivity function $\sigma(f)\begin{cases} \approx 0 & \text{if} \quad f \gg c \\ \gg 0 & \text{if} \quad f \approx c \end{cases}$ where c is a *target level* ($= -0$ for phase stability test)

Local growth assumption $\hat{x} \equiv$ any local minima then in a small neighbourhood $B_r(\hat{x})$ of radius r

$$[f(\hat{x} + \rho s) - f(\hat{x})] = \rho^p[f(\hat{x} + s) - f(\hat{x})]$$

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As a particular choice of σ we choose

$$\sigma(f) = \frac{1}{(f-c)^{2e+1}} \text{ with } e \approx \frac{1}{p}$$

Resulting ODE $\ddot{x}(t) = -\nabla\phi(x(t))$ with

$$\phi(x(t)) = \begin{cases} -\dfrac{1}{2e(f-c)^{2e}} & \text{if} \quad e > 0 \\ \ln(f-c) & \text{if} \quad e = 0 \end{cases}$$

Theorem (Griewank, 1981) $x_0 \in B_r(\hat{x})$, $\dot{r}_0 = \dot{x}_0^\top (x_0 - \hat{x})$

$$\dot{r}_0 \leqslant 0 \;\wedge\; c < f(\hat{x})\,,\, ep \leqslant 1 \Longrightarrow \text{divergence}\,,$$

$$\dot{r}_0 \geqslant 0 \;\wedge\; c \geqslant f(\hat{x})\,,\, ep \geqslant 1 \Longrightarrow f(x(\tau)) \longrightarrow c\,.$$

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$$\dot{r}_0 \geqslant 0 \;\wedge\; c \geqslant f(\hat{x})\,, ep \geqslant 1 \Longrightarrow f(x(\tau)) \longrightarrow c\,.$$

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Hamiltonian systems

The ODE can be rewritten in following Hamiltonian form
$\dot{x} = v = \nabla_v H(x, v)$, $\dot{v} = -\nabla_x H(x, v)$, where

$$H(x, v) = \frac{1}{2}\|v\|^2 + \phi(x)$$

$$\Longrightarrow \; H(x(t), v(t)) = H_0 = \frac{1}{2}\|v_0\|^2 + \phi(x_0) \; \forall t \in [0, \infty) \, .$$

$$\Longrightarrow \; \|v_0\| = \frac{1}{\sqrt{e}(f-c)^e} \text{ if } H_0 = 0.$$

Another invarient of the symplectic flow $\Phi_t : (x_0, v_0) \mapsto (x(t), v(t))$ is the volume $|\Phi_t(S)| = |S|$ and projections onto $(x(t), v(t))$ planes are constant.

$$(\Phi_t')^\top J(\Phi_t') = J \, , \text{where } J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} .$$

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Optimization problem

- The ODE is discretized using the mid-point rule, which is a symplectic integrator, and the next step at any point is calculated as an unconstrained and regularized minimization problem.
- The Hessian for this minimization problem has the form

$$B_k = \alpha_k I + \beta_k \nabla^2 f(x_k) + \gamma_k \nabla f(x_k) \nabla f^\top (x_k) \, .$$

- α_k, β_k and γ_k change drastically from step to step.
- Solved using a quasi Newton method.

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Linear Algebra Tasks

- Updating Eigenvalue factorizations

$$B_k = Q_k \Sigma_k Q_k^\top \text{ with } Q_k^\top Q_k = I$$

- Subject to
  - rescalings.
  - rank one updates.
  - shifts by multiples of identity.
- Everything with $\mathcal{O}(n^2)$ effort.
- Trummer problem solved in principle.

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