2025

UNVEILING THE MAGIC OF MIDSTREAM INNOVATION

GPA MIDSTREAM CONVENTION

Welcome!

Flow Regime Modelling of Demethanizer Reboiler using Lattice Boltzmann Method CFD

Enhanced Physics Modelling for Multi-Component, Multi-Phase, Thermal Flows

Jack A. Smith, P.E., MSME
Chem Eng Ph.D. Candidate

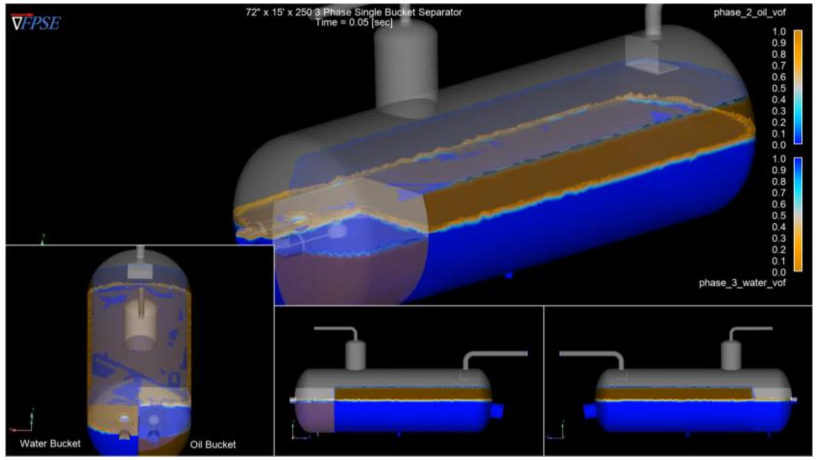
FPSE
Fluid & Power
Systems Engineering

UTSA
The University of Texas at San Antonio™

Presentation Layout

- Objective: Present Lattice Boltzmann Method CFD
  - Details of multi-component, multi-phase, thermal flows for O&G
- Discussion Topics
  - Natural Gas Liquids (NGLs) & Thermosiphon Reboiler Loop
  - Two-Phase Flow & Flow Regimes
  - Computational Fluid Dynamics (CFD)
    - Continuum Naiver-Stokes CFD
    - Lattice Boltzmann Method CFD
  - General Graphics Processing Units (GPUs)

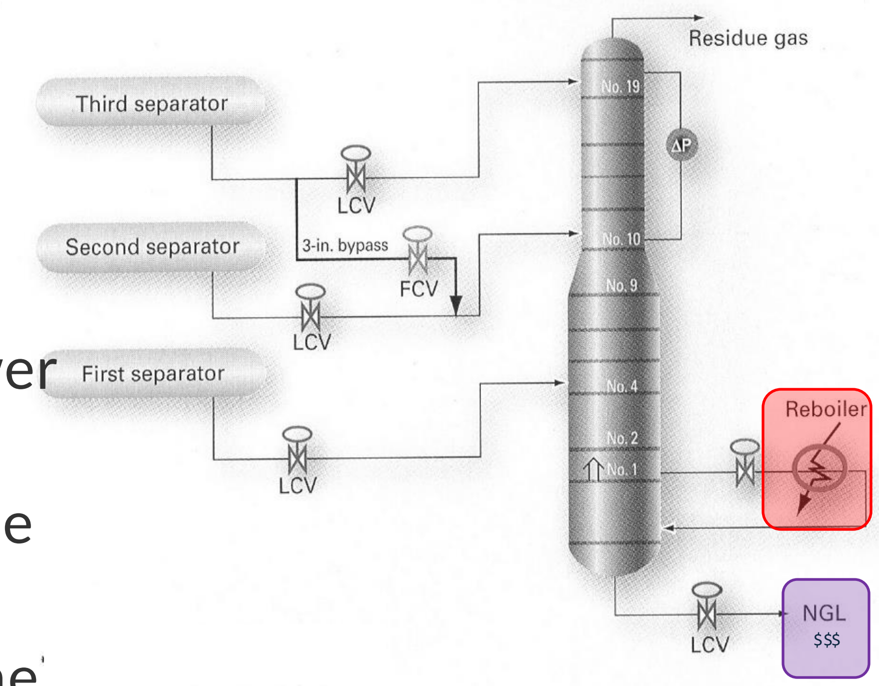
Pipestone Cryogenic Sour Gas Processing Plant.
SOURCE: NS Energy website



Double Bucket 3-Phase Separator CFD
SOURCE: FPSE, LLC

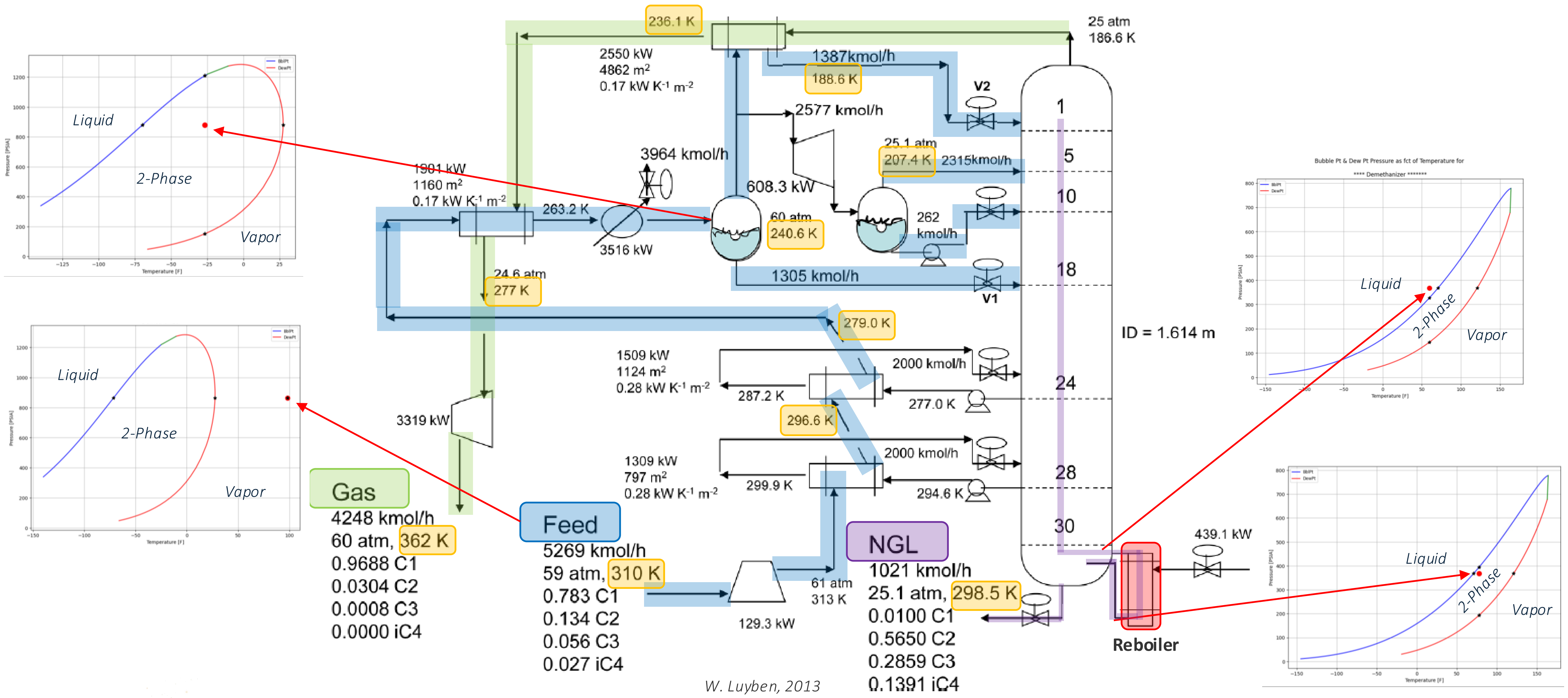
Natural Gas Liquids (NGLs)

- NGLs are lucrative HC fluids in oil & gas processing
- NGLs consist of C_2+ or C_3+ hydrocarbons
- Cryogenic gas plants process a raw NG stream & recover NGLs via a series of distillation processes
- 1st process is a cryogenic high-pressure Demethanizer tower where CH_4 is separated from the NGLs
- Thermosiphon loop often used instead of pump system due to low cost & simplicity
- Thermosiphon reboiler loop design is challenging due to the presence of multiple species in a multi-phase flow
- Improperly designed thermosiphon reboiler loop can lead to flow regime transitioning & reboiler loop stall



Demethanizer Tower

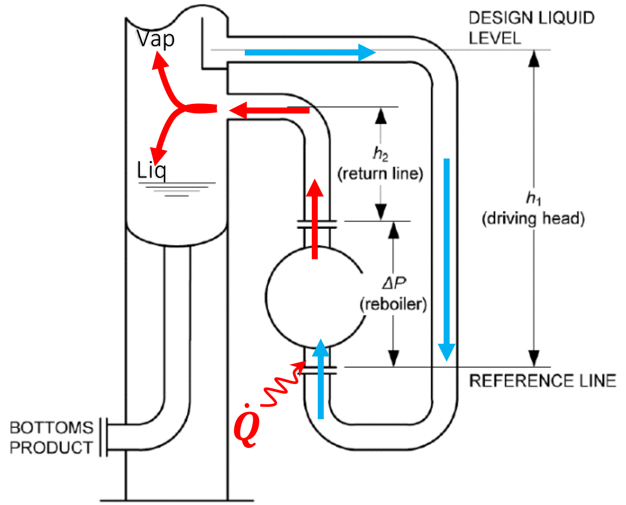
Demethanizer Flow Sheet



W. Luyben, 2013

Thermosiphon Loop & Reboiler

- Sat or Sub-cooled liq from bottom tray routed to reboiler
  - Reboiler boils out C_1 and/or C_2, forming a two-phase mixture
  - $\rho_{2phz} < \rho_{satliq}$
  - $\rho_{satliq} g h_1 > (\rho_{2phzgh2}$ + Reboiler ΔP + Return Piping ΔP)
- Thermosiphon loop is a complex process
  - Fluid dynamics
  - Conduction and convection heat transfer
  - Nucleate & pool boiling
  - Miscible, Multi-Component Vapor-Liquid Equilibrium (VLE)
- Brazed Aluminum Heat Exchanger (BAHX)
  - Temperature & Pressure fluctuations due to flow regime transitioning believed to cause BAHX fin fatigue failures
  - There is a need to understand what's occurring within the BAHX



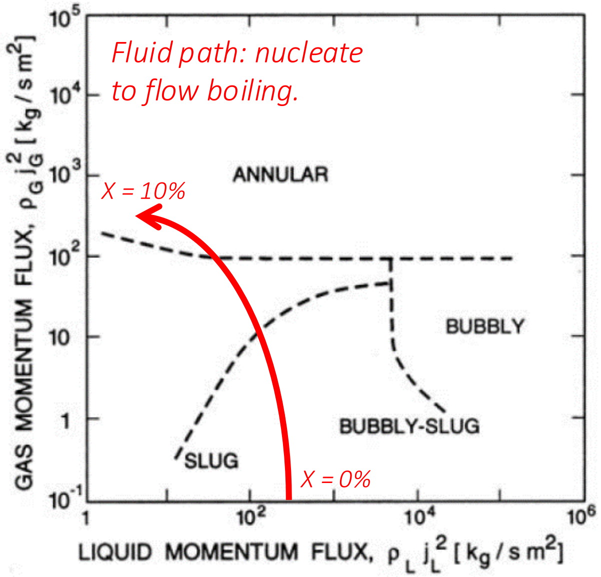
Thermosiphon Loop with Reboiler

CHART Industries BAHX

Two-Phase Flow & Flow Regimes

- Two-phase flow:
  - Vapor & Liquid co-flow with an interface between the phases
  - Flow develops into one of several "flow regimes"
  - Each regime has a distinct, visual morphology
  - The flow often passes through several regimes
  - Regime depends on vapor & liquid fluxes & surface tension
  - Heat, mass xfer, & momentum exchange occur at the phase interface
  - Annular flow preferred to maximize wall heat transfer for phase change
- Flow regime maps aide the design of piping systems
  - Approach is +50 yrs old
  - Similar maps in GPSA Engineering Data Book dating back to the 70's
  - Maps are generally qualitative based on visual morphology
- Better tools needed for effective, trouble-free thermosiphon design
  - Avoid flow regime transitioning: intermittent annular – to slug – to annular flow
  - "Virtual P&T sensors" via CFD can provide a view into the HX passages
  - Parametric CFD to determine size of the operating window

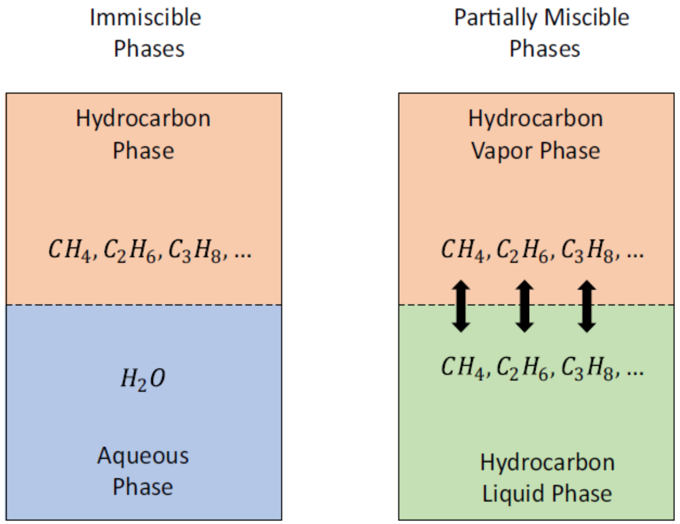
Two-Phase Vertical Flow. L-R: Bubbly, Cap-Bubbly, Slug, Churn, Annular, Ishii and Hibiki, 2006.



Hewitt and Roberts Vertical Flow Map (1969).

Multi-Component Phase Interaction

- Immiscible phases: No molecular level mixing
- Partially miscible phases: Molecular level mixing
- The thermosiphon loop involves a partially miscible system
- Inlet composition affects the vapor & liquid compositions via chemical potential, & this affects vapor density
- Iso-fugacity used to determine phase compositions: $f_{i,v} = f_{i,l}$



Soomro, 2023.

Continuum, Two-Fluid Multiphase CFD

- Navier-Stokes Equations (NSE)
- General Two-Fluid Model (TFM)

Set of eqns is difficult to program and converge

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{\boldsymbol{V}}_k) = \sum_{j=1}^{\Pi} (\dot{m}_{jk} - \dot{m}_{kj}) + S_k$$

Continuity eqn,
α_k is vol fraction of k^{th} phase,
S_k is source term

$$\frac{\partial}{\partial t}(\alpha_k \rho_k \vec{\boldsymbol{V}}_k) + \nabla \cdot (\alpha_k \rho_k \vec{\boldsymbol{V}}_k \vec{\boldsymbol{V}}_k) = -\alpha_k \nabla P + \nabla \cdot (\alpha_k \bar{\bar{\boldsymbol{\tau}}}_k) + \alpha_k \rho_k \vec{\boldsymbol{g}} + \sum_{j=1}^{n} \left(K_{jk}(\vec{\boldsymbol{V}}_j - \vec{\boldsymbol{V}}_k) + \dot{m}_{jk} \vec{\boldsymbol{V}}_{jk} - \dot{m}_{kj} \vec{\boldsymbol{V}}_{kj} \right) + \sum_{q=1}^{r} \vec{\boldsymbol{F}}_{kq}$$

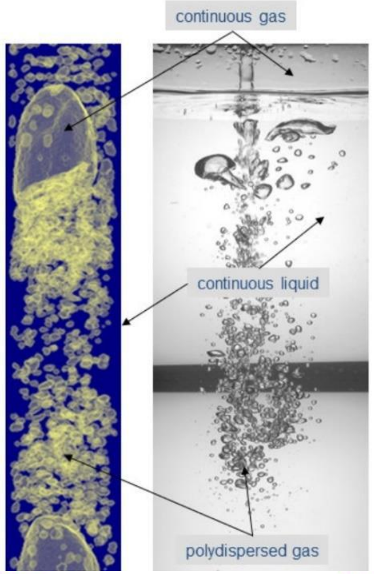
NS Momentum eqn,
K_{jk} is momentum exchange coef,
$\vec{F}_{kq}$ is the q^{th} external force on the k^{th} phase

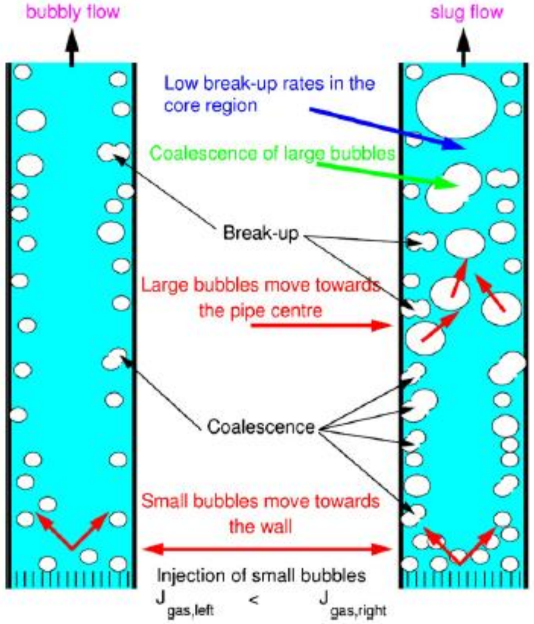
$$\frac{\partial}{\partial t}(\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k \vec{\boldsymbol{V}}_k h_k) = \nabla \cdot \left(\alpha_k k_{eff,k} \nabla T_k - \sum_{l=1}^{q} h_{lk} \vec{J}_{lk} + \bar{\bar{\boldsymbol{\tau}}}_{eff,k} \cdot \vec{\boldsymbol{V}}_k \right) + \sum_{j=1}^{n} (\dot{Q}_{jk} + \dot{m}_{jk} h_{jk} - \dot{m}_{kj} h_{kj}) + S_k$$

Energy eqn,
k_{eff} is thermal conductivity,
h_k is enthalpy of k^{th} phase
J_{lk} is diffusive flux of species l into the k_{th} phase,
$\dot{Q}_{jk}$ is heat xfer

ANSYS FLUENT GENTOP

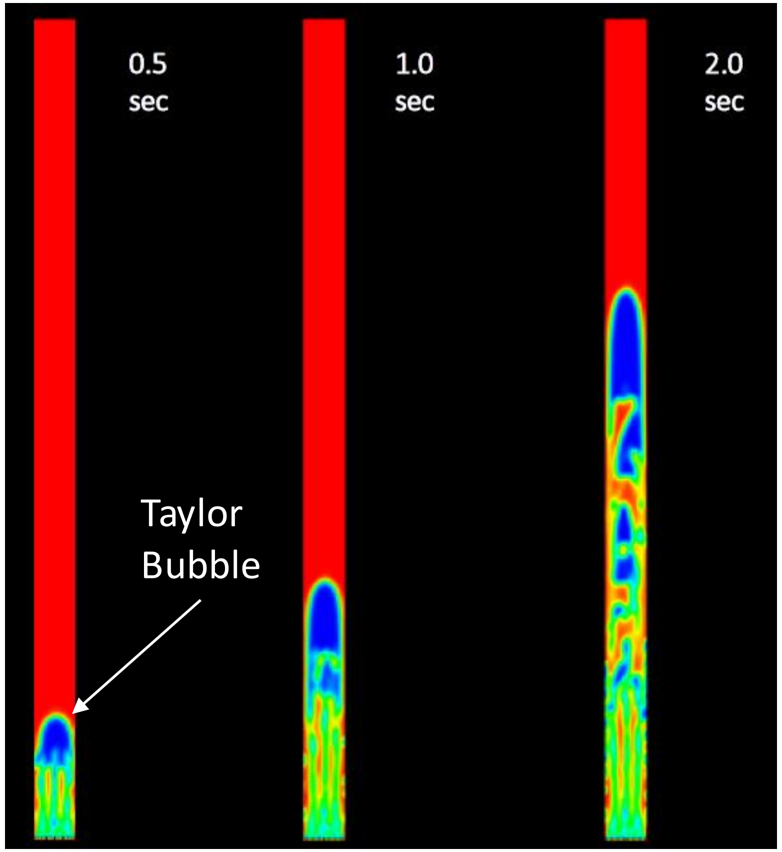
- Generalized Two-Phase Flow Model (GENTOP)
  - Flow regime transition model for single component, isothermal flows
- 3-Field, 2-Fluid model
  - Field 1: Continuous liquid phase, fluid 1
  - Field 2: Continuous vapor phase, fluid 2
  - Field 3: Subgrid vapor phase of polydisperse bubbles, fluid 2
  - Polydisperse means “many sizes” of bubble diameters
    - User specifies range of diameters to model a priori
    - Bubbles interact with other bubbles & the continuous vapor phase
    - User specifies nucleation, growth, aggregation, & breakage models
  - Phases interacts with through empirical interfacial closure models
- Developed basis air-water system experiments





FLUENT GENTOP Example

- CH_4 bubbles (blue) co-flowing with C_3H_8 liquid (red) in a 12" pipe, 20 ft long
  - CH_4 Superficial Velocity = 10 ft/s (vapor)
  - C_3H_8 Superficial Velocity = 3 ft/s (liquid)
  - Taylor bubble formation is predicted
  - Immiscible & No interphase mass transfer
- GENTOP lacks:
  - Real-gas EoS for two phase flow
  - Multi-component VLE
  - Wall boiling
  - These models exist in FLUENT, but not incorporated in GENTOP
  - Models can be added/modified using UDFs
- GENTOP not yet mature for Thermosiphon Loop



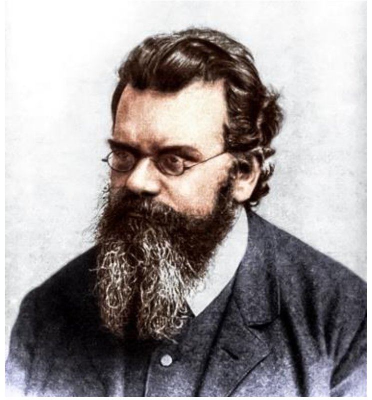
Lattice Boltzmann Method CFD

- A mesoscale method based on the kinetic theory of gases & Boltzmann distribution

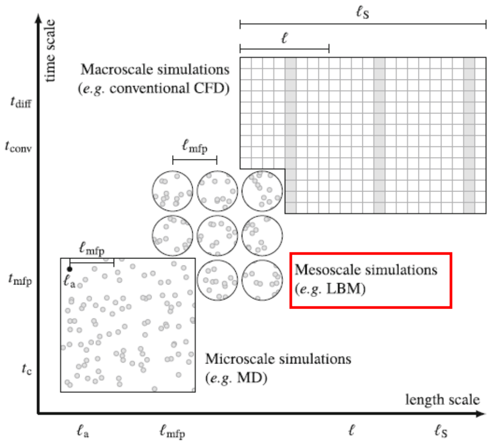
$$f = \frac{\rho}{(2\pi RT)^{D/2}} exp\left[-\frac{\left(\vec{\xi}-\vec{u}\right)^2}{2RT}\right] \quad (continuous)$$

Maxwell-Boltzmann Distribution

- Mesoscale lies between molecular modelling and continuum modelling
- Tracks a “collection” of particles moving on a lattice at discrete velocities
- Weakly compressible method, inherently allows for density gradients
- Less memory intensive than molecular modelling
- “Truer” physics than continuum CFD and avoids empirical closure models
- LBM not as intuitive as continuum CFD
- Boundary conditions not as “direct” as continuum CFD
- LBM is highly parallelizable on the GPU
- Advances in GPU technology propelling LBM CFD



Ludwig Boltzmann: 1844-1906



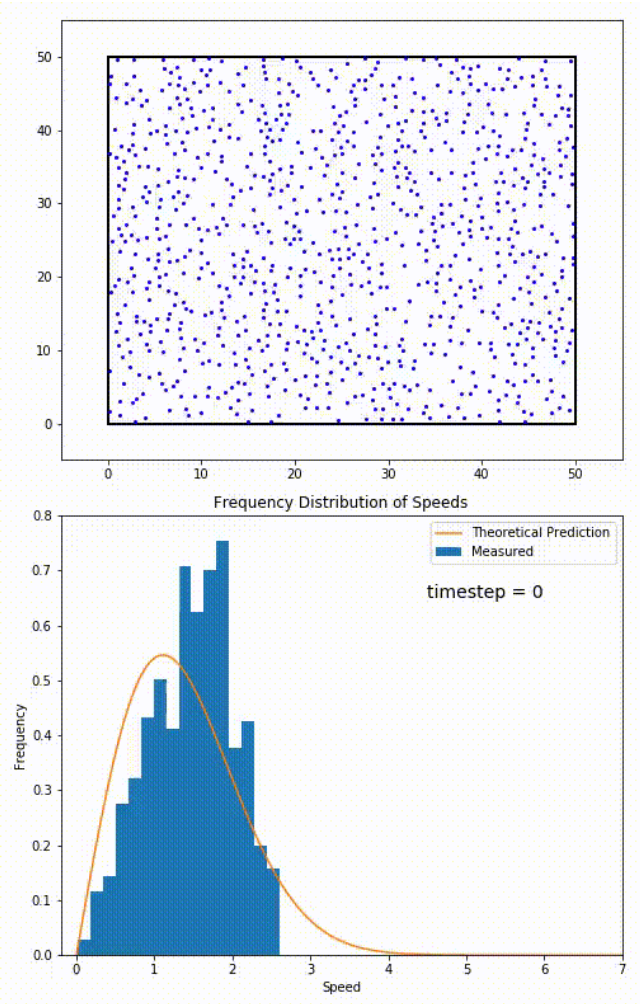
Relative Length Scales of Computational Models

Kinetic Theory of Gases & LBM CFD

- LBM CFD simulates the Boltzmann Transport Equation (BTE)

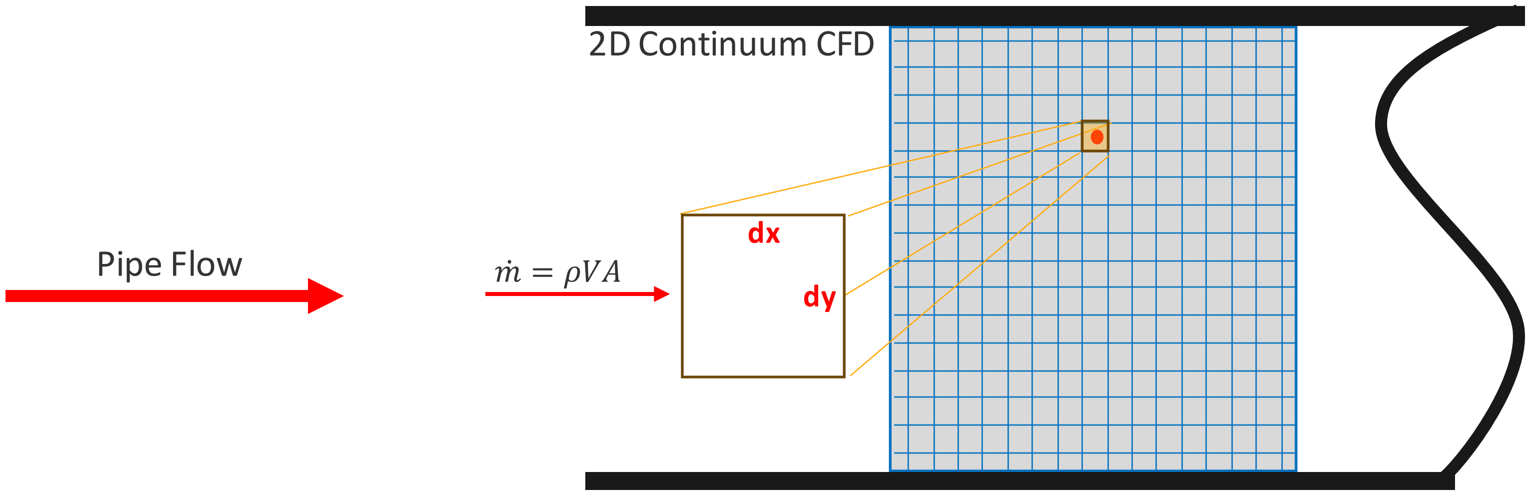
$$\frac{df(\vec{x},\vec{\xi},t)}{dt} = \frac{\partial f}{\partial t} + \xi_\alpha \frac{\partial f}{\partial x_\alpha} + \frac{F_\alpha}{\rho}\frac{\partial f}{\partial \xi_\alpha} = \Omega(f) \longleftarrow \textit{BTE}$$

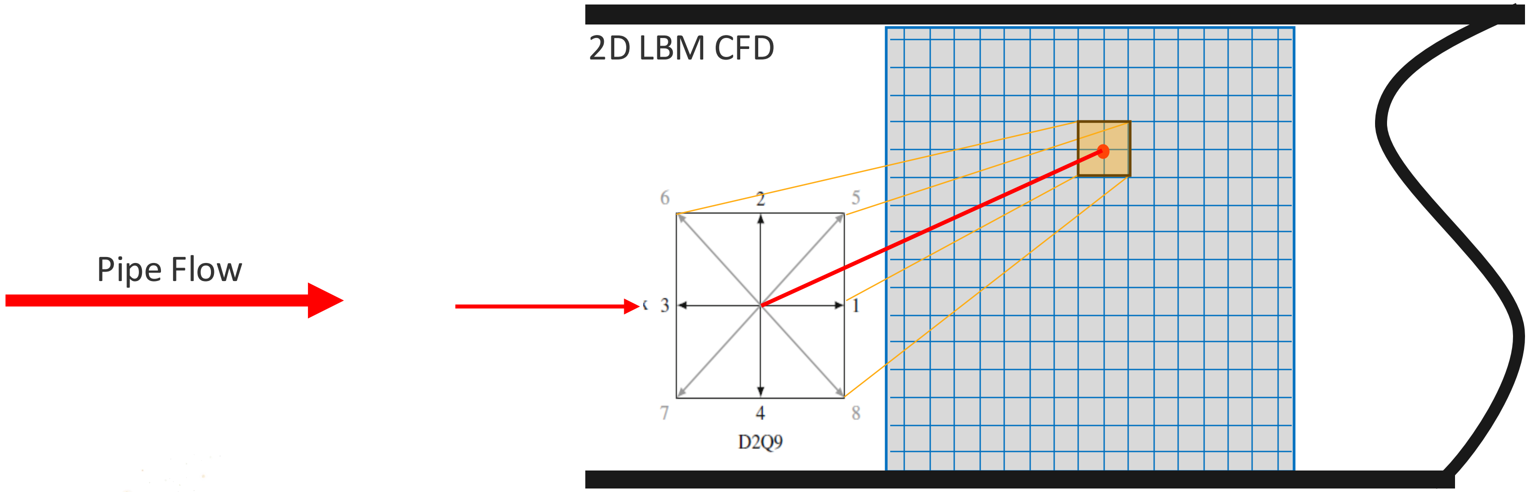
- Tracks the evolution of the Particle Distribution Function (PDF), $f(\vec{x},\vec{\xi},t)$
  - “Collections” of particles stream & collide on a lattice at “discrete” velocities
  - Generalization of density in 3d physical space and 3d velocity space
  - LBM “indirectly” solves the Continuity, NSEs, & Energy eqn
- Forcing functions add physics to LBM
  - Vapor and liquid phases form “naturally”
  - No empirical closure models or surface tracking required
  - Liquid-Solid interaction naturally carried out with surface potential function
- Energy equation solved with separate PDF

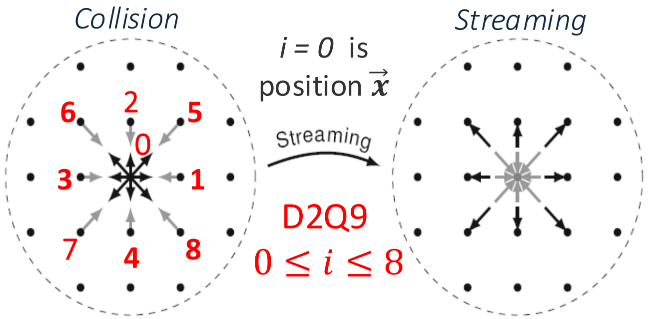


WIKIPEDIA: “Maxwell-Boltzmann Distribution”

Continuum & LBM CFD







Evolution & Discretization of the PDF

Advected f

Body forces acting on f

Particle velocity, ξ_α

Collision Operator, Relaxation to equilibrium e.g. BGK

f is the particle distribution function

$$\frac{df(\vec{x},\vec{\xi},t)}{dt} = \boxed{\frac{\partial f}{\partial t}} + \boxed{\xi_\alpha \frac{\partial f}{\partial x_\alpha}} + \boxed{\frac{F_\alpha}{\rho}\frac{\partial f}{\partial \xi_\alpha}} = \Omega(f)$$

Evolution of the ***continuous*** *Boltzmann eqn*

$$\boxed{f_i(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) - f_i(\vec{x},t)} = [\Omega_i(\vec{x},t) + \vec{F}_i(\vec{x},t)]\Delta t$$

c_i are discrete lattice velocities

Evolution of the ***discrete*** *Boltzmann eqn. Fwd Euler.*

Set of eqns is easier to program and converge. No ∇P & no non-linear advection $\vec{U}\cdot\nabla\vec{U}$ to solve.

The collision step can be done for all lattice nodes at 1 time on a GPU. Same for streaming step.

$$\boxed{f_i^*(\vec{x},t)} = f_i(\vec{x},t) - \left(\frac{f_i(\vec{x},t) - f_i^{eq}(\vec{x},t)}{\tau}\right)\Delta t + \left(1 - \frac{1}{2\tau}\right)\vec{F}_i(\vec{x},t)\Delta t \quad (collision)$$

$$f_i(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = \boxed{f_i^*(\vec{x},t)} \quad (streaming)$$

Macroscopic Variables Easily Computed

$\rho(\vec{\boldsymbol{x}}, t) = \sum_i f_i$ and $\vec{\boldsymbol{u}}(\vec{\boldsymbol{x}}, t) = \frac{1}{\rho}\left[\sum_i f_i\, \vec{\boldsymbol{c}}_{\boldsymbol{i}} + \frac{\vec{\boldsymbol{F}}\Delta t}{2}\right]$

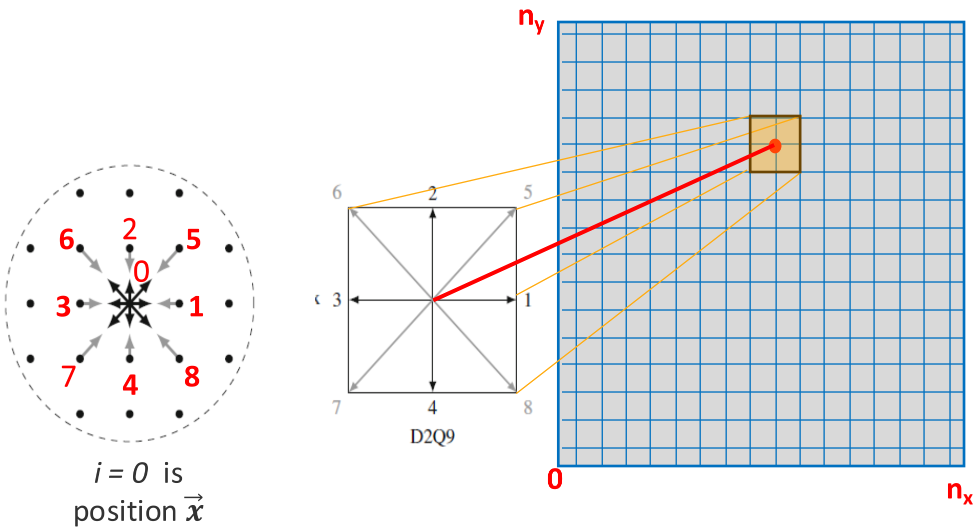
The macroscopic density and velocity.
The solution to the NSE.

For D2Q9 Velocity Set

$$\rho(\vec{\boldsymbol{x}}, t) = f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + f_8$$

$$u_x(\vec{\boldsymbol{x}}, t) = \frac{(f_1+f_5+f_8)-(f_3+f_6+f_7)}{\rho(\vec{\boldsymbol{x}},t)} + \frac{[(F_1+F_5+F_8)-(F_3+F_6+F_7)]\Delta t}{2\rho(\vec{\boldsymbol{x}},t)}$$

$$u_y(\vec{\boldsymbol{x}}, t) = \frac{(f_2+f_5+f_6)-(f_4+f_7+f_8)}{\rho(\vec{\boldsymbol{x}},t)} + \frac{[(F_2+F_5+F_6)-(F_4+F_7+F_8)]\Delta t}{2\rho(\vec{\boldsymbol{x}},t)}$$



Forcing Functions

- Forcing functions are “extensions” of the standard LBE
- Forcing functions are body forces on the fluid
- Forcing functions include
  - Vapor-Liquid interface, $\vec{\boldsymbol{F}}_{i,vl}$
  - Solid-Liquid interface, $\vec{\boldsymbol{F}}_{i,sl}$
  - Gravity body force, $\vec{\boldsymbol{F}}_{i,B}$
- Easily incorporated into the standard LBM equation

$$\vec{\boldsymbol{F}}_i = \vec{\boldsymbol{F}}_{i,vl} + \vec{\boldsymbol{F}}_{i,sl} + \vec{\boldsymbol{F}}_{i,B}$$

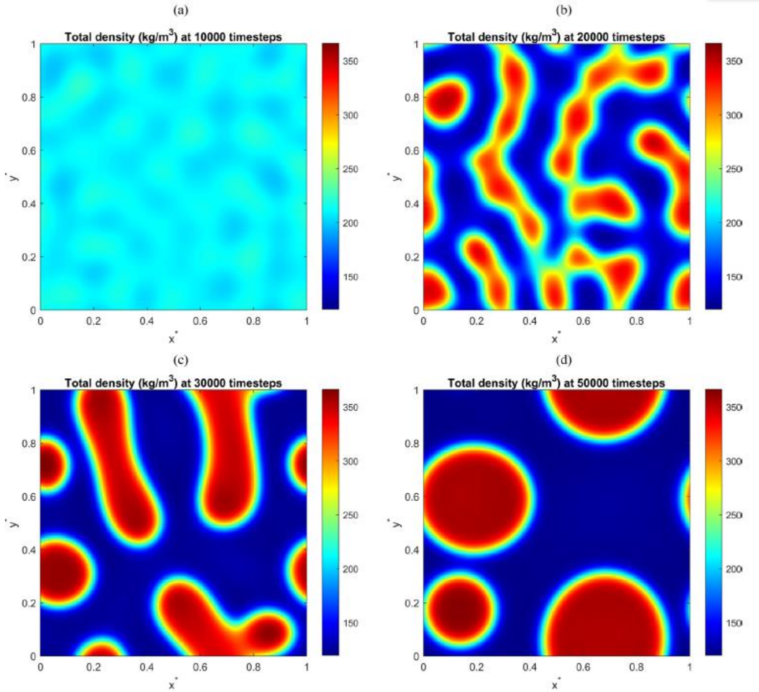
$$f_i(\vec{\boldsymbol{x}} + \vec{\boldsymbol{c}}_i \Delta t, t + \Delta t) - f_i(\vec{\boldsymbol{x}}, t) = \left[\Omega_i(\vec{\boldsymbol{x}}, t) + \vec{\boldsymbol{F}}_i(\vec{\boldsymbol{x}}, t)\right]\Delta t$$

Multi-Component Interphase Force

- Interphase force is generated by fugacity gradient and gradient of the Laplacian of density for the “k^{th}” component
- Derived via isothermal Gibbs-Duhem relation & chemical potential
- Free Energy model ensures thermodynamic consistency
- Vapor and Liquid phases develop naturally
- No interface tracking or closure models required
- Interphase force composed of bulk fluid & interface components for each component “j”

$$\vec{\boldsymbol{F}}_{\boldsymbol{i,j}}\Big|_{\boldsymbol{vl}} = \underbrace{-\tilde{\rho}_j RT\nabla \ln f_j}_{\text{Bulk Fluid}} + \underbrace{\tilde{\rho}_j \sum_{k=1}^{N_C} \nabla\left(\sqrt{k_j k_k \nabla^2 \tilde{\rho}_k}\right)}_{\text{Interface}} \quad (isothermal)$$

- Demonstrated spinodal decomposition for mixtures with up to 10 components
- Flow regimes expected to naturally develop
- Needs to be expanded for non-isothermal case



Soomro’s isothermal fugacity based multi-component VLE LBM simulating spinodal decomposition, 2023.

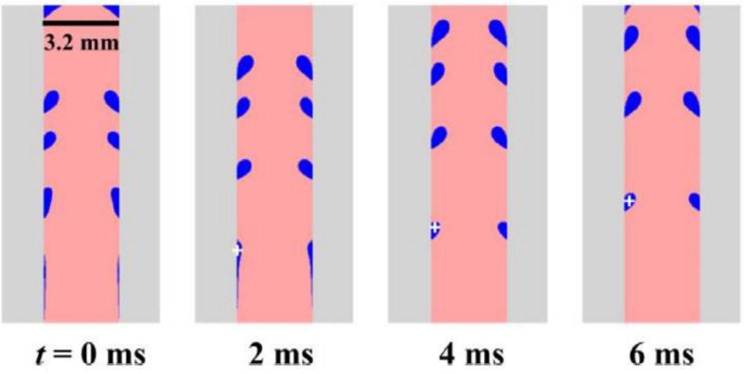
Solid-Liquid Interaction & Buoyancy Forces

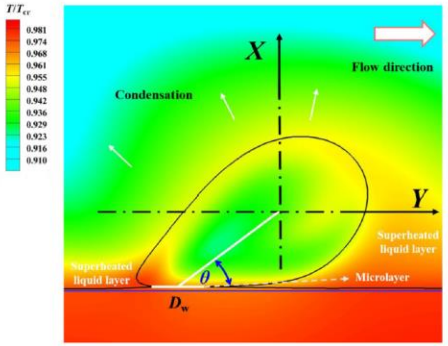
- SL interaction and boiling pseudo-potential interaction force

$$\vec{F}_{i,j}\Big|_{sl} = -\left(1 - e^{-\rho(\vec{x},t)}\right)\sum_i g_s\, w_i s(\vec{x} + \vec{c}_i\Delta t)\cdot \vec{c}_i\Delta t$$

- g_s is the SL interaction force strength, controlling wettability, or contact angle
- Separate Temperature PDF solved for energy equation
- Bubbles form naturally, depart, and rise
- Bubble nucleation, departure diameter, departure frequency, and rise velocity agree well with experimental correlations independently developed by Fritz, Kocamustafaogullari, & Phan
- Gravity force driven buoyancy

$$\vec{F}_j\Big|_B = \vec{G}(\rho_j(\vec{x},t) - \rho_{avg})$$

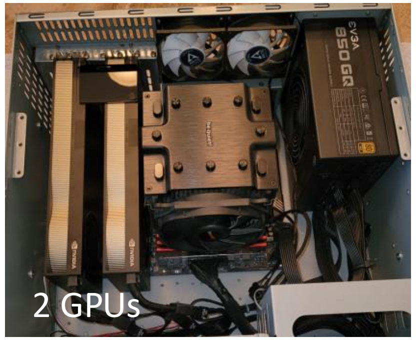


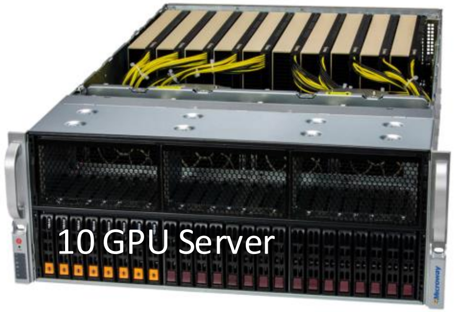


Chen, et. al, "Experimental and LBM simulation study on the bubble dynamic behaviors in subcooled flow boiling", 2023.

General GPUs

- Designed for parallelization & speed
- Can be “stacked” in desktops, servers, & super clusters
- Ideal platform for LBM CFD
- All LBM lattice nodes updated ≈simultaneously

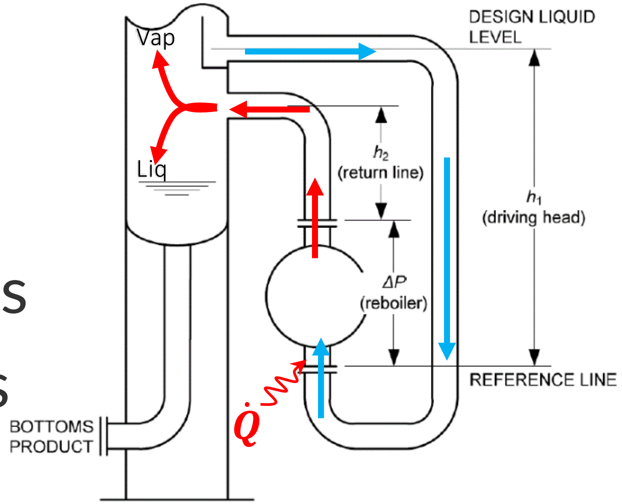

2 GPUs


10 GPU Server

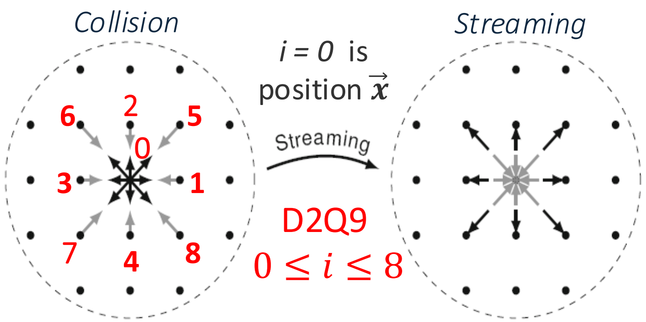

XAI: 200,000 GPUs

Conclusions

- Advances in GPU technology enable LBM CFD development
- Programming ease & parallelization offset physics complexity
- Continuum CFD models rely on experimental closure relations
- LBM CFD models don't rely on experimental closure relations
- Forcing functions extend generic LBM CFD solver
- Currently expanding models for non-isothermal case & integrating for industrial applications
- Thermosiphon Reboiler Loop analysis planned



Thermosiphon Loop with Reboiler



Thank you!

Questions?