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Phase Change with Convection: A Reference Solution

by

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$\boxed{\textbf{Solution methods}}$

in Heat Transfer and Fluid Flow

- **Analytical** $\Longrightarrow$ Limited in scope
- **Experimental** $\Longrightarrow$ Expensive, slow
- **Numerical**

1. Cheap
2. Powerful
3. General
4. Unlimited output
5. Extended parameter range

Numerical Methods

$\Longrightarrow$ Risk of errors

- Formulation
- Discretization
- Language
- syntax

$\Longrightarrow$ Need for code verification

- Experimental results (not recommended)
- Known analytical solutions
- Benchmark (reference) solutions

Benchmark Solutions

⟹ Heat Transfer

- Heat Transfer + convection: **M. Hortman, M. Peric, and G. Sheuerer**,*"Finite Volume Multi-grid Prediction of Laminar Natural Convection: Benchmark Solutions"*, IJNMF, vol. 11, pp. 189–207, 1990.

⟹ Phase change

- Analytical solutions available for 1-D and 2-D Stefan problems: **V. Alexiades and A. D. Solomon**, *Mathematical Modeling of Melting and Freezing Processes*, 1993.

⟹ Phase change + convection

- No reference solution
  1. **D. Gobin and P. Lequere**, *Melting from an Isothermal Vertical Wall: Synthesis of a Numerical Comparison Exercise*, CAMES, vol. 7, pp. 289–306, 2000.
  2. **I. Wintruff, C. Günther, and A. G. Class**, *interface-tracking control-volume finite-element method for melting and solidification problems - Part II: verification and application*, NHT Part B, vol.39, pp.127–149, 2001.

Present Study

$\Longrightarrow$ Topic

- Focus on the tin melting problem with $Pr = 0.02$, $St = 0.01$, $Ra = 2.5 \times 10^5$.

$\Longrightarrow$ Work To Be Done

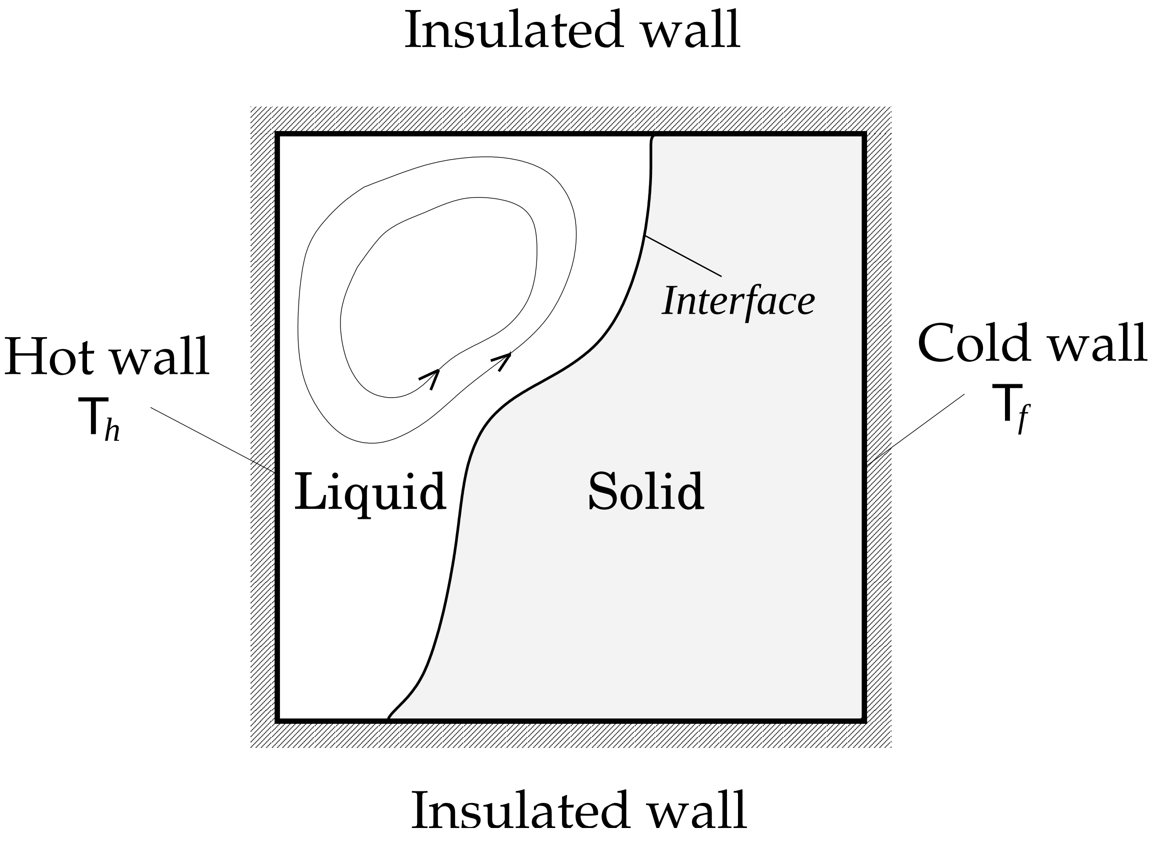
- Enthalpy model for phase change
- Effect of grid size
- Heat Transfer and Fluid Flow parameters

$\Longrightarrow$ Purpose

- Assess grid convergence level
- Obtain a reference solution

Tin Melting Problem

`P. Lequere & D. Gobin` "*Melting driven by natural convection, a comparison exercise: first results.*" International Journal of Thermal Sciences, Vol 38 (1999) pp. 5-26.



- Two-dimensional square cavity filled with tin.
- Initially, tin is solid at freezing temperature T_f.
- At time $t = 0$, the left wall is heated to a temperature T_h above the melting temperature.

Mathematical Model

Basic assumptions

- Navier-Stokes equations.
- Two-dimensional, unsteady, .
- Cartesian coordinates.
- Conservative u-v-P formulation.
- Incompressible fluid with Boussinesq approximation.
- Constant thermophysical properties (μ, c_p, λ, β).
- Equal thermophysical properties for solid and liquid.

Phase change

- One domain formulation: ENTHALPY METHOD.
- Cavity material: POROUS medium ⟶ Darcy's law.
- Porosity obeys Karman-Kozeny law.
- Pure material (isothermal phase change).

Mathematical Model

Mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0$$

Momentum

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho \vec{V} u) = \nabla \cdot (\mu \nabla u) - \frac{\partial P}{\partial x} - Au$$

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho \vec{V} v) = \nabla \cdot (\mu \nabla v) - \frac{\partial P}{\partial y} - Av + \rho_{\text{ref}} g \beta (h - h_{\text{ref}})/c_p$$

Energy

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \vec{V} h) = \nabla \cdot (\alpha \nabla h) - \frac{\partial \rho \Delta H}{\partial t} - \nabla \cdot (\rho \vec{V} \Delta H)$$

Enthalpy and liquid fraction

$$H = h + \Delta H \qquad h = cT \qquad f_L = \frac{T - T_S}{T_L - T_S}$$

$$\Delta H = \begin{cases} L & \text{if } T \geq T_L \\ f_L L & \text{if } T_L > T \geq T_S \\ 0 & \text{if } T_S > T \end{cases}$$

Source terms

$$A = -\frac{C(1 - f_L)^2}{f_L^3 + q}$$

C and q are constants.

t : Time
x,y : Cartesian coordinates
u,v : x and y Components of velocity vector $\vec{V}$.
ρ : Density
P : Pressure
T : Temperature
h : Enthalpy per unit volume
c_p : Specific heat per unit mass
λ : Thermal conductivity
α : λ/c_p
μ : Dynamic viscosity
g : Gravity
β : Coefficient of thermal expansion
ΔH : Latent heat of the control volume
L : Latent heat per unit mass
T_L : Liquidus temperature
T_S : Solidus temperature
f_L : Liquid fraction
ref : Subscript indicating reference values.

The velocity vector $\vec{V} = (u, v)$ is the ensemble averaged velocity (or superficial velocity). The actual velocity of the liquid $\vec{V_l}$ (our model assumes a fixed solid matrix : zero solid velocity) is related to $\vec{V}$ through the relation $\vec{V} = f_L \vec{V_l}$.

Numerical Method

Space Discretization

- Finite-volume.
- Staggered grid for velocities.
- Second order accuracy

Time discretization

- Euler implicit ⟶ First order accuracy.

Coupling and nonlinearity

- `SIMPLER` algoritm (Patankar 1980).

Linear systems

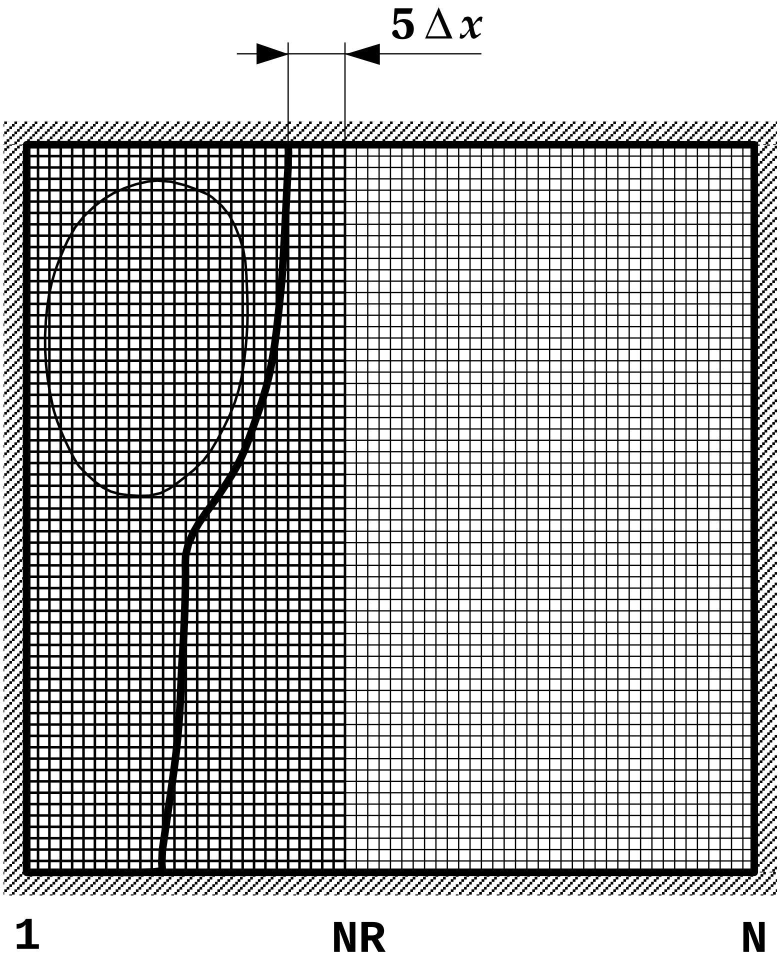
- `BICGSTAB-SIP` : u, v, h, P (nonsymmetric).
- `CG-SSIP` : P', ψ (symmetric).

Liquid fraction update

- `Brent, Voller and Reid` 1988:

$$\Delta H^{k+1} = \Delta H^{k} + \omega_{\Delta H} \frac{a_P^h}{a_P^{oh}} \left\{ h^k - c_p \left[\frac{T_L - T_S}{L} \Delta H^k + T_S \right] \right\}$$

Computational Grid



- All equations, including energy equation, are solved in a reduced domain containing the liquid
- Boundary of reduced domain is located 5 Δx away from the solid-liquid interface
- Consequence ⟶ Large savings in `CPU` time and disc space for data ouput

A Grid Convergence Study

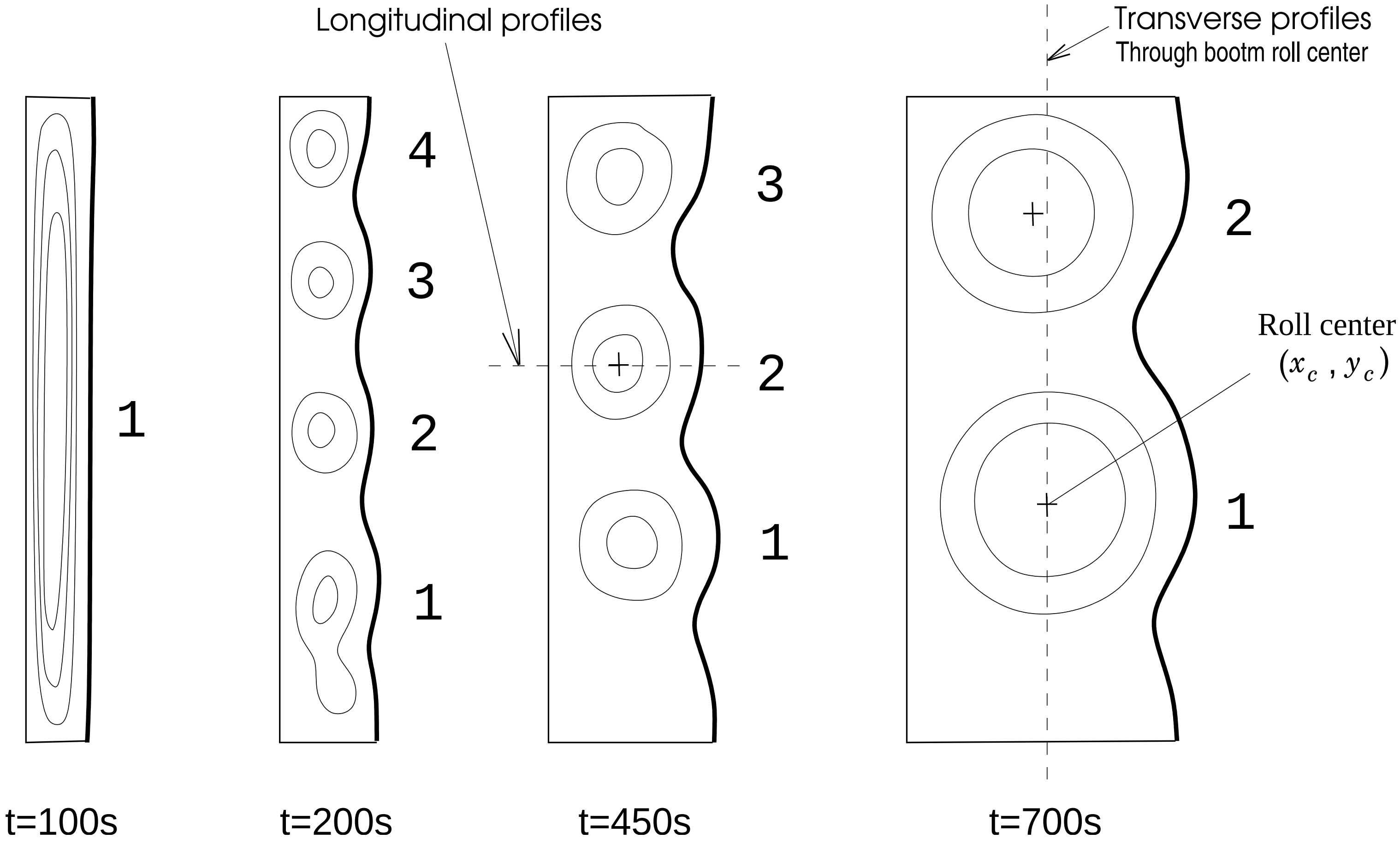
Procedure

- Grid refinement
- Grids 50×50 up to 800×800
- Effect on several parameters

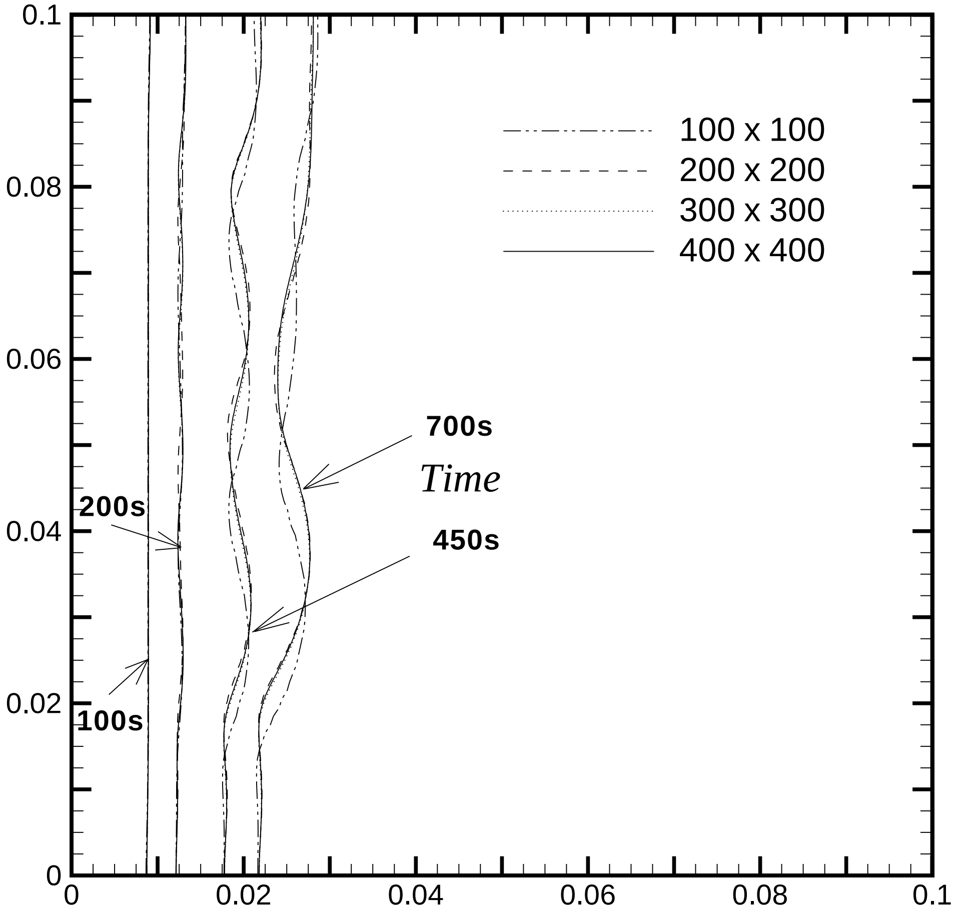
Purpose

- Reach convergence.
- Assess the convergence level
- Propose a reference solution

Flow patterns - Physics of the problem



Solid liquid interface



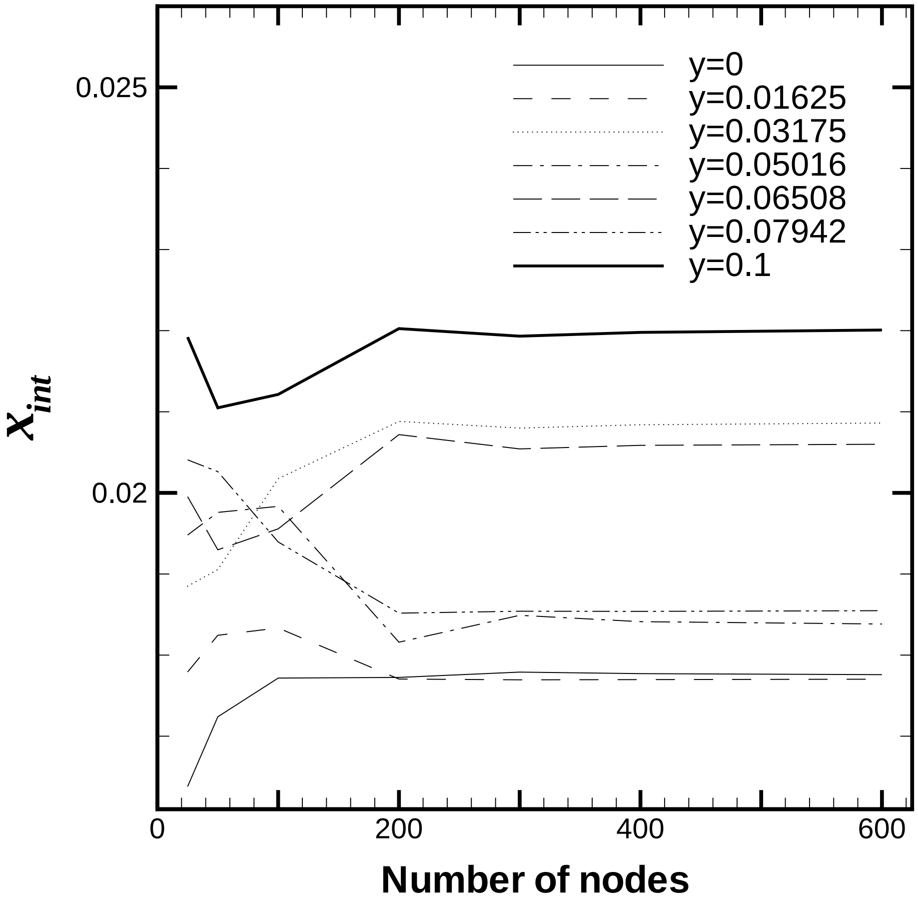
- Flat interface at $t = 100s$.

- Wavy interface at later times.

- Error on x_{int} is .1% at $t = 200s$, .5% at $t = 450s$, and 1% at $t = 700s$.

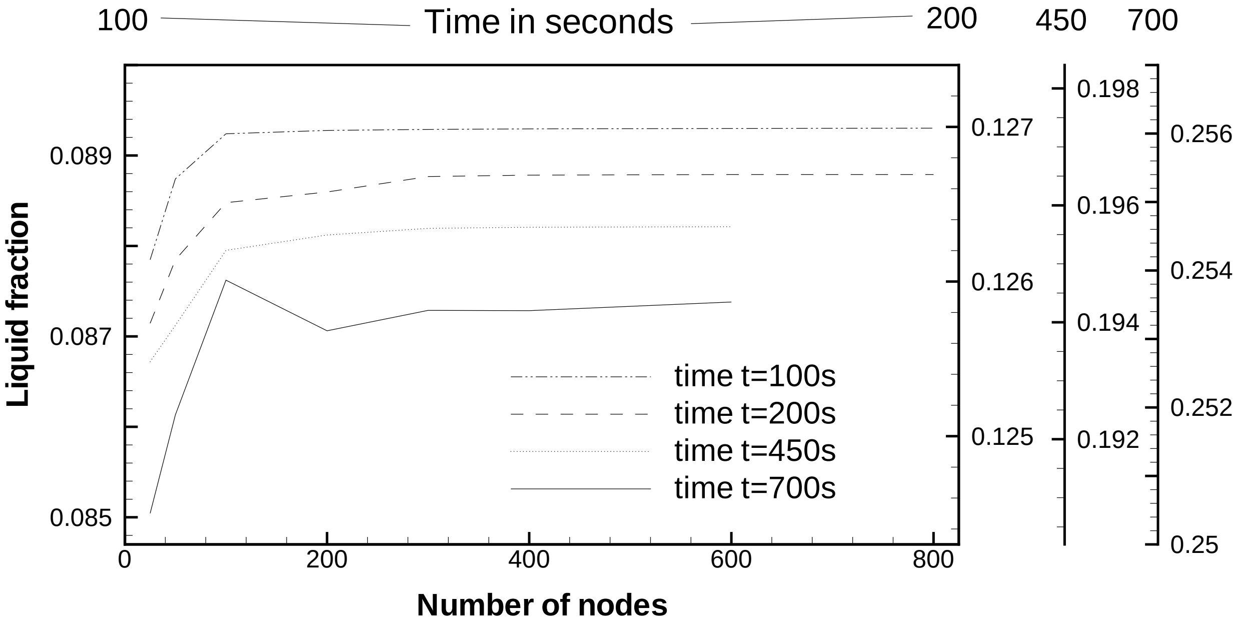
Trough and crests locations

at Time $450s$



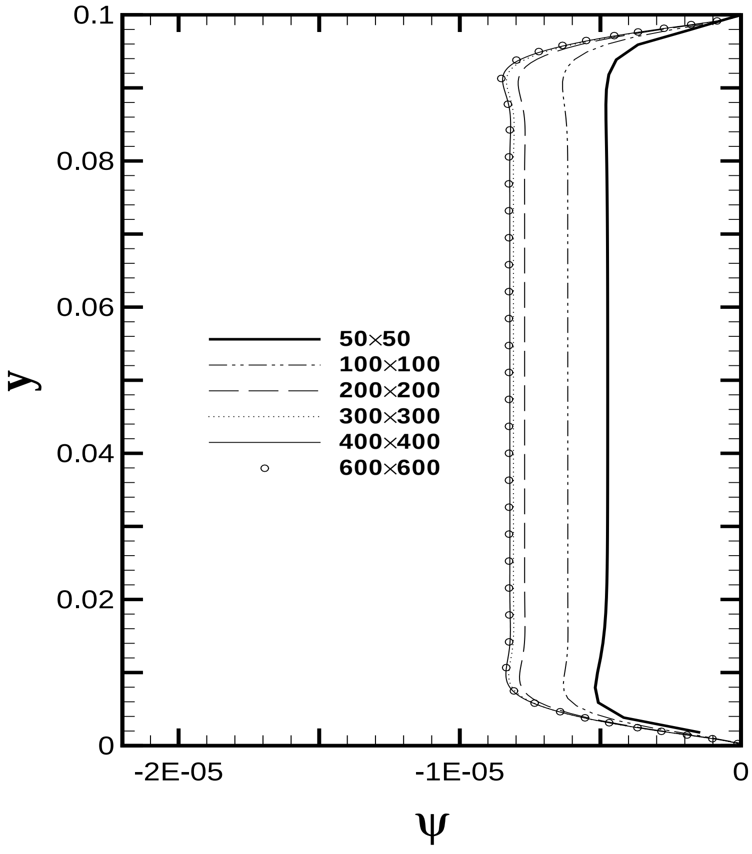
- Convergence within 0.5%

Total liquid fraction

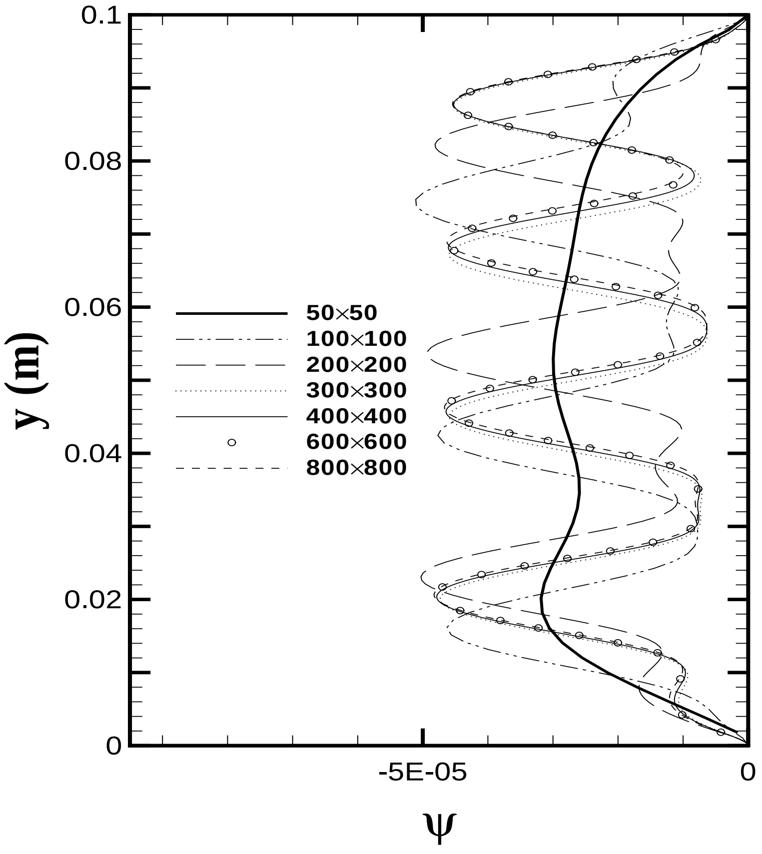


- Convergence within 0.01%

Transverse Profiles of Streamfunction

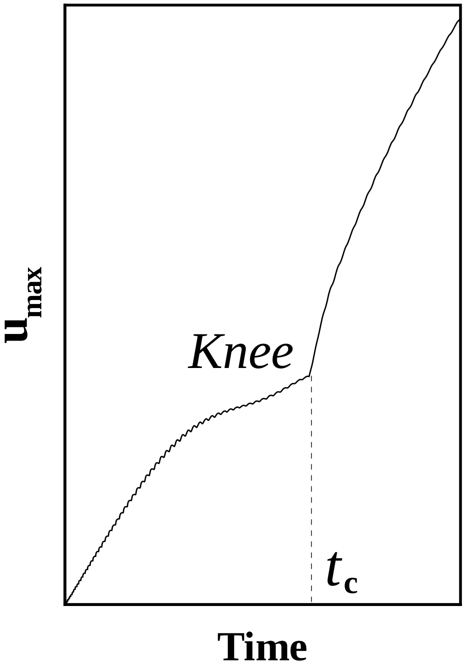


$t = 60s$

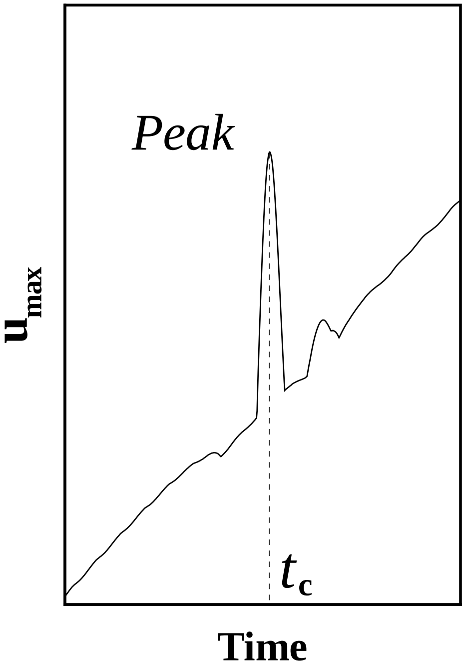


$t = 200s$

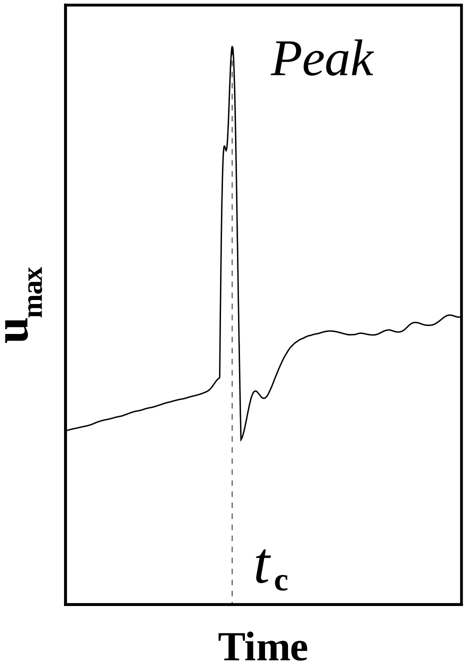
Bifurcation and roll-merging times



Onset of 4 rolls

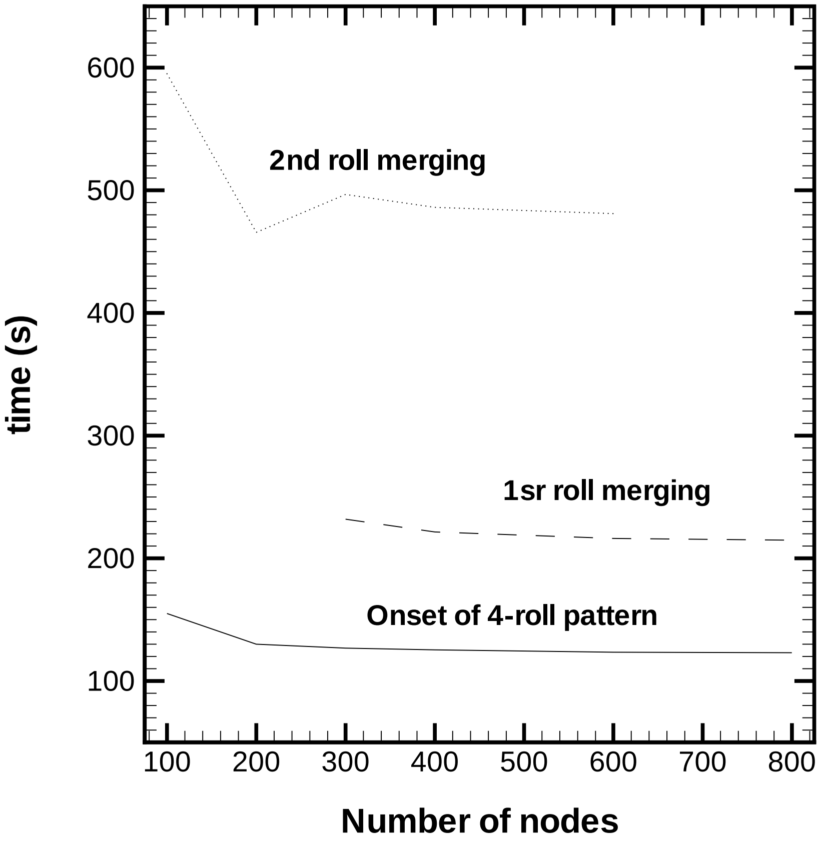


1st roll Merging



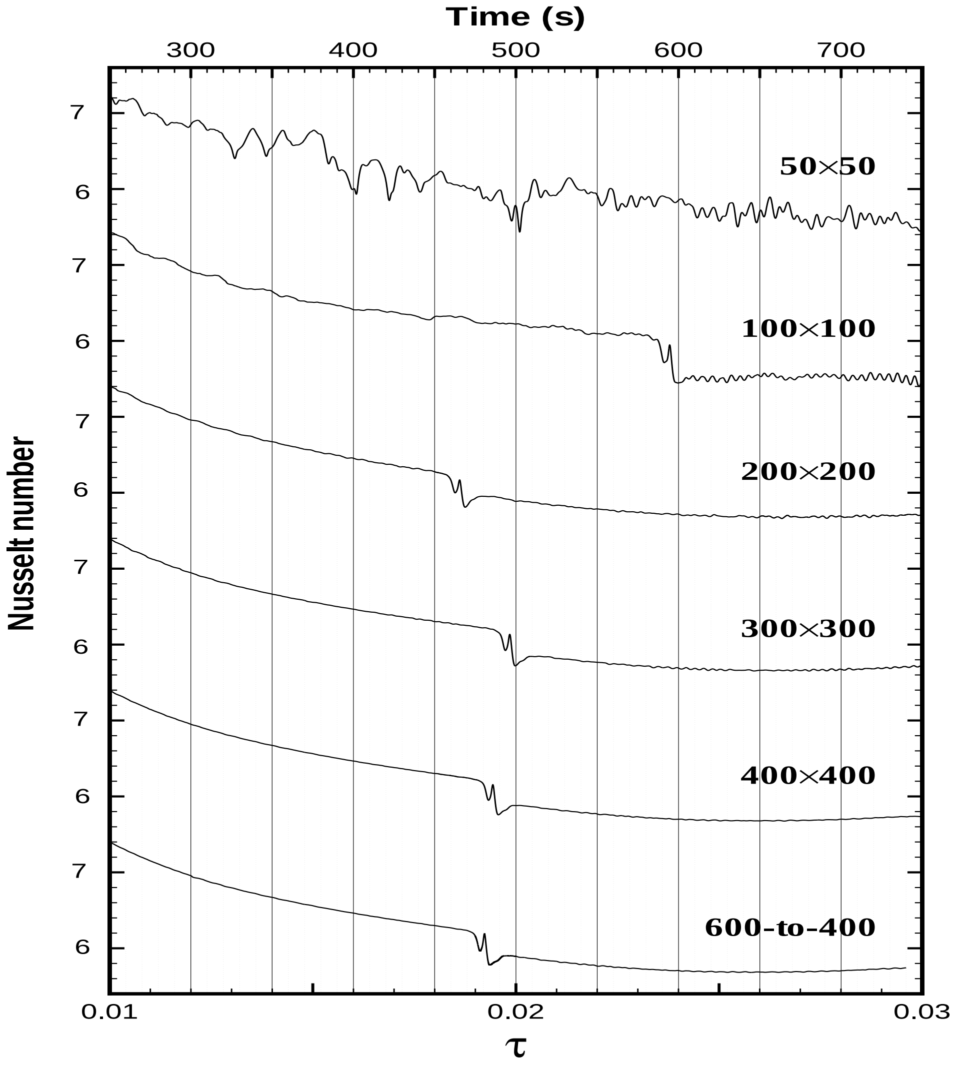
2nd roll merging

Bifurcation/Roll-Merging Times



- 2nd order convergence.
- Error within 0.01%.

Nusselt number at hot wall



- Good convergence of mean value
- Oscillations disappear as mesh is refined
- Merging time grid dependent

A Reference Solution

Tables

- Transverse profiles of T, ψ, u, v.
- Interface location
- Liquid fraction
- Nusselt number
- Roll center parameters
- bifurcation and roll merging times

Plots

- ψ_{min} and ψ_{max} versus time
- Nusselt number versus time
- Liquid fraction versus time
- 2-D contours of all variables
- Time evolution of flow parameters at three selected locations.

CPU Times

Grid	**Time (sec)**	**CPU (hr)**	**Machine**
$\mathbf{100 \times 100}$	0–700	20	SUN Enterprise 6000
$\mathbf{200 \times 200}$	0-700	260	CRAY SV1
$\mathbf{400 \times 400}$	0-700	450	Compaq Alphaserver SC clusters
$\mathbf{600 - to - 400}$	0-700	1070	Compaq Alphaserver SC clusters
$\mathbf{600 \times 600}$	0-500	2500	Compaq Alphaserver SC clusters
$\mathbf{800 \times 800}$	0-225	1750	Compaq Alphaserver SC clusters

Future Directions

⟹ Improve accuracy.

- Higher order methods
- Adaptive mesh refinement.
- Parallelization.

⟹ Validate the model.

- Reported discrepancies between numerics and experiments.
- Change the model.
- Adjust experiments.

Conclusion

⟹ **Outcome of the work**.

- Solution is converged to 0.01% for many variables.
- Some parameters are accurate to within 1% only.
- A reference solution is proposed (numbers and plots).

⟹ **Necessity for further work**.

- Improve on accuracy.

Acknowledgment

We are gratefull to Oak Ridge National Laboratory for their amazingly fast Compaq Alphaserver SC clusters, without which this study could not have been carried out.