Parareal algorithm for two phase flows simulation

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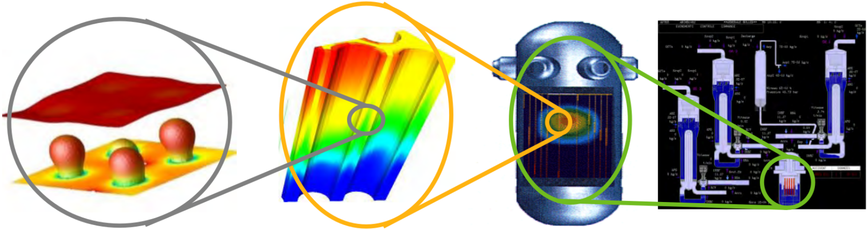
Outline

1. Context and model
2. Cathare numerical scheme
3. Numerical results

Outline

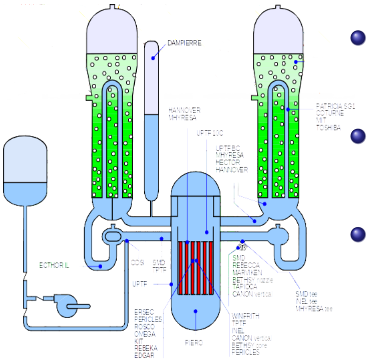
Different scales of modelling

Two-phase flow models (gas-liquid flows) used in the simulation of boiling in the cooling system of a nuclear power plant.



Direct numerical Simulation - Meso-scale - Component scale - System scale

Motivation



Code for **A**nalysis of **TH**ermalhydraulics during **A**ccident and for **R**eactor safety **E**valuation

- Cathare essentially simulates assemblies of 1D (pipes) and 3D elements (vessels)
- Typical cases involve up to 10^2 or 10^3 cells with 3D elements and involve up to a million of numerical time steps
- Space domain decomposition method is implemented and allows a speed-up of about 4-8 using 10-12 processors
- Strategy of time domain decompositions, complementing the space domain decomposition, based on the **parareal method**

Six equation model

Fine physical phenomena (description of the interfaces) are filered by the model.

Flow is dominated by convection. Neglecting the viscous effects, we obtain:

$$\begin{cases} \partial_t(\alpha_k\rho_k) + \partial_x(\alpha_k\rho_k u_k) = \Gamma_k \\ \partial_t(\alpha_k\rho_k u_k) + \partial_x(\alpha_k\rho_k u_k^2) + \alpha_k\partial_x p = \alpha_k\rho_k g + F_k^{\text{int}} \\ \partial_t\left[\alpha_k\rho_k\left(H_k + \frac{u_k^2}{2}\right)\right] + \partial_x\left[\alpha_k\rho_k u_k\left(H_k + \frac{u_k^2}{2}\right)\right] = \alpha_k\partial_t p + \alpha_k\rho_k u_k g + Q_k^H \end{cases}$$

Main unknowns: (p, α_1, u_k, H_k), with $\alpha_1 + \alpha_2 = 1$ and ρ_k are computed thanks to equations of state: $\rho_k = \rho_k(p, H_k)$

Γ_k, Q_k^H: mass and energy transfers between phases

F_k^{int}: interfacial forces

Closure laws

- Tabulated equation of state with polynomial interpolation (IAPWS)
- Closure laws in the momentum equations:
  - Well posedness of the system

    M. Ndjinga, A. Kumbaro, F. De Vuyst, P. Laurent-Gengoux, Influence of Interfacial Forces on the Hyperbolicity of the Two-Fluid Model
  - Interfacial friction in Cathare depends on the flow regime (bubbly, annular, dispersed,..) and on the geometry:

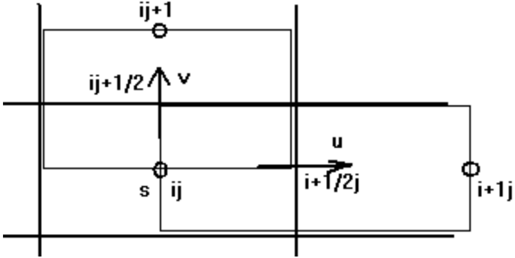
$$\tau_i = f(\alpha_1, \sigma, \rho_1, \rho_2, \mu_1, \mu_2, D_h)(u_1 - u_2)^2$$

    Damping term to avoid the increase of the relative velocity $u_r = u_1 - u_2$.

Outline

Cathare scheme

- Simulate the components of a reactor thanks to a semi-heuristic approximation of the six-equation model
- Staggered mesh
  - with scalar variables (p, H_k, α) at cell centers
  - normal vector (u_k) at edges
- Fully implicit numerical scheme



Time discretisation

Neglect mass and energy transfers between phases

$$\begin{cases} \dfrac{(\alpha_k\rho_k)^{n+1}-(\alpha_k\rho_k)^n}{\Delta t}+\partial_x(\alpha_k\rho_k u_k)^{n+1}=0 \\ \dfrac{(\alpha_k\rho_k u_k)^{n+1}-(\alpha_k\rho_k u_k)^n}{\Delta t}+\partial_x(\alpha_k\rho_k u_k^2)^{n+1}+\alpha_k^{n+1}\partial_x p^{n+1}=(\alpha_k\rho_k)^{n+1}g+F_k^{n,n+1} \\ \dfrac{1}{\Delta t}\left[(\alpha_k\rho_k)^{n+1}\left(H_k+\dfrac{u_k^2}{2}\right)^{n,n+1}-(\alpha_k\rho_k)^n\left(H_k+\dfrac{u_k^2}{2}\right)^{n-1,n}\right] \\ +\partial_x\left[\alpha_k\rho_k u_k\left(H_k+\dfrac{u_k^2}{2}\right)\right]^{n+1}=\alpha_k^{n+1}\dfrac{p^{n+1}-p^n}{\Delta t}+(\alpha_k\rho_k u_k)^{n+1}g \end{cases}$$

Space discretisation

Upwind scheme to express cell centered unknowns at edges in mass and energy equations.

$$(\alpha_k^U)_{i+1/2} = \begin{cases} (\alpha_k)_i - 10^{-5} \ , (u_k)_{i+1/2} > 0 \\ (\alpha_k)_{i+1} - 10^{-5} \ , (u_k)_{i+1/2} < 0 \end{cases}$$

$$(\rho_k^U)_{i+1/2} = \begin{cases} (\rho_k)_i \ , (\alpha_k^U)_{i+1/2}(u_k)_{i+1/2} > 0 \\ (\rho_k)_{i+1} \ , (\alpha_k^U)_{i+1/2}(u_k)_{i+1/2} < 0 \end{cases}$$

The convection term:

$$(u_k \partial_x u_k)_{i+1/2} = \begin{cases} (u_k)_{i+1/2}((u_k)_{i+1/2} - (u_k)_{i-1/2}) \ , (u_k)_{i+1/2} > 0 \\ (u_k)_{i+1/2}((u_k)_{i+3/2} - (u_k)_{i+1/2}) \ , (u_k)_{i+1/2} < 0 \end{cases}$$

Semi-heuristic approach: if $(u_k)_{i+1/2} \leq (u_k)_{i-1/2}$ and $(\alpha_k)_i \leq 10^{-3}$ then:

$$(u_k \partial_x u_k)_{i+1/2} = (u_k)_{i+1/2} \left((u_k)_{i+1/2} - \frac{C_1(\alpha)(u_k)_{i-1/2} + C_2(\alpha)(u_k)_{i+1/2}}{C_1(\alpha) + C_2(\alpha)} \right)$$

Non linear solver

Newton scheme:

The semi-discretised problem: $\dfrac{U^{n+1}-U^{n}}{\Delta t}+A(U^{n+1},U^{n})=S(U^{n})$

$$\frac{\Delta U^{k+1}}{\Delta t}+J(U^{k+1},U^{k})\Delta U^{k+1}=S(U^{n},U^{k}),\text{ where: }\Delta U^{k+1}=U^{k+1}-U^{k}$$
$$\text{and : }U^{k+1}=(P^{k+1},\alpha_V^{k+1},H_l^{k+1},H_v^{k+1},u_l^{k+1},u_v^{k+1})$$

- In Cathare: By Gauss elimination, obtain a system with pressure increment only. Solve the problem in pressure with a direct linear solver (LAPACK BLAS)
- In MiniCathare (Cathare restricted to 1 test case): solve the complete linear system with an iterative linear solver (PETSC library)

Characteristics of Cathare scheme

- Accuracy of the scheme for nearly incompressible flows
- For single phase flows:
  - Riemann solvers have poor precision in the incompressible limit

    S. Dellacherie, Analysis of Godunov type schemes applied to the compressible Euler system at low Mach number
  - Staggered schemes enjoy good precision at the incompressible limit
- Two phase flows:
  - Special treatment of the vanishing phase

    M. Ndjinga, T. P. K. Nguyen and C. Chalons, A 2x2 hyperbolic system modelling incompressible two phase flows: theory and numerics
  - Countercurrent flows

Outline

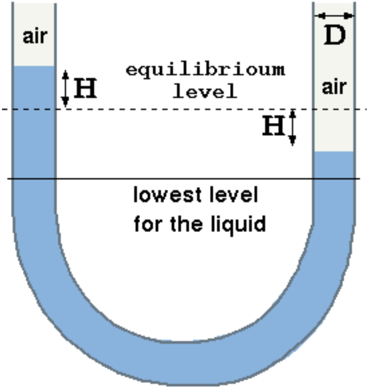
Oscillating manometer

G.F. Hewitt, J.M. Delhaye, N. Zuber, Multiphase science and technology

Ability of a scheme to preserve system mass and to retain the gas-liquid interface

Flow regime: separated phases

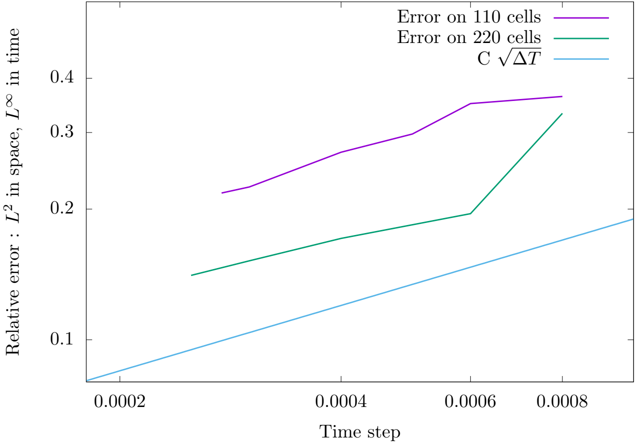
Interfacial friction term to handle the vanishing phase and adaptation of the convection term



Stopping criteria

- Initial condition: $P = 10^5$, $h_l = 4.17 \times 10^5$, $h_v = 2.68 \times 10^6$, $u_v = u_l = -2.1$ and
$$\alpha_v = \begin{cases} 1 - 10^{-5}, \text{ in the upper half} \\ 10^{-5}, \text{ elsewhere} \end{cases}$$
- Time interval : [0,20]
- Order of convergence in time of the Cathare scheme:
    - Reference solution: 220 cells and $\delta t = 10^{-5}$
    - Error norm: $\frac{max_n||U^n - U^n_{ref}||_{L^2}}{max_n||U^n_{ref}||_{L^2}}$ where $U^n = (P^n, \alpha^n_v, h^n_v, h^n_l, u^n_v, u^n_l)$

Order of convergence in time



D. Bouche , J.-M. Ghidaglia , F. Pascal, Error estimate and the geometric corrector for the upwind finite volume method applied to the linear advection equation

Parareal for hyperbolic equations

J.-L. Lions , Y. Maday , G. Turinici , Résolution par un schéma en temps "pararéel"

Initialisation: $k = 0$, $U_{n+1}^0 = G(T_n, T_{n+1}, U_n^0)$ *sequential*

Parareal iteration k: $(U_n^k)_{n=0}^N$ *known.*

(k.1) Compute fine solution on each $]T_n, T_{n+1}[$ *:*

$$F(T_n, T_{n+1}, U_n^k) \quad \textit{in parallel}$$

(k.2) Prediction coarse step: $G(T_n, T_{n+1}, U_n^{k+1})$ *sequential*

(k.3) Correction step:

$$U_{n+1}^{k+1} = G(T_n, T_{n+1}, U_n^{k+1}) + F(T_n, T_{n+1}, U_n^k) - G(T_n, T_{n+1}, U_n^k)$$

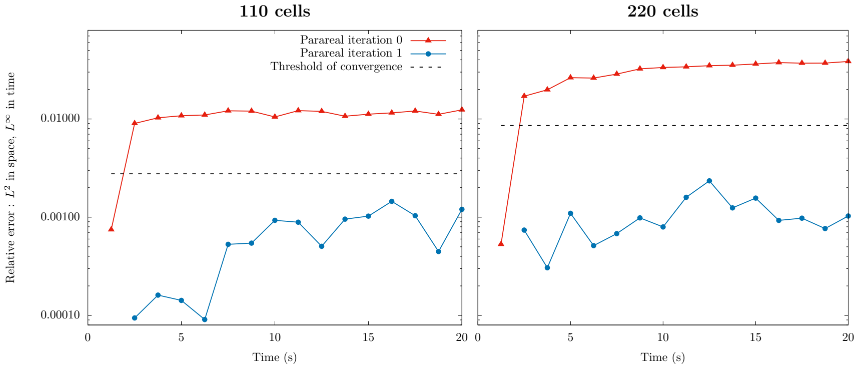
- Convergence properties [Gander, Vandewalle, 2007] and stability analysis [Maday, Ronquist, Staff, 2005]
- Dependence on the regularity of the initial condition and solution [Bal, 2005] and [Dai, Maday, 2013]
- Correction procedure re-using previously computed information based on a projection on a Krylov subspace [Gander, Petcu, 2008] or on a reduced basis [Chen, Hesthaven, Zhu, 2014] .
- Coarsening in space [Ruprecht, 2014] and [Lunet, 2017]

Coarse and fine solvers

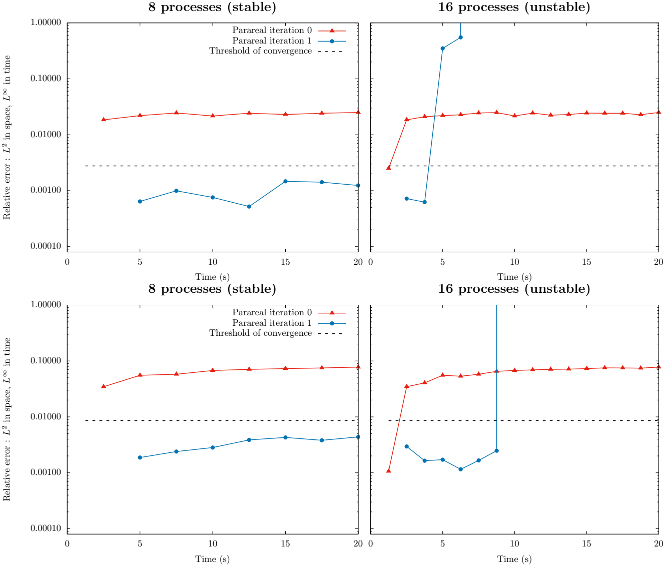
- Coarse and fine solvers share the same physics and mesh
- Two tests :
  - 110 cells: $\Delta t_{coarse} = 2.5 \times 10^{-4}$ and $\delta t_{fine} = 10^{-5}$
  - 220 cells: $\Delta t_{coarse} = 2 \times 10^{-4}$ and $\delta t_{fine} = 10^{-5}$
- An unstable example: Mesh of 110 cells, $\Delta t_{coarse} = 4 \times 10^{-4}$ and $\delta t_{fine} = 10^{-5}$ with 8 time windows (stable) and 16 time windows (unstable)

Numerical convergence

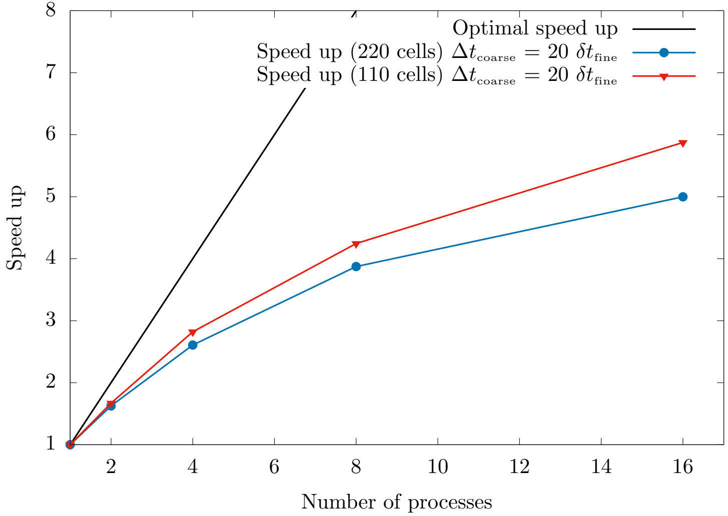
16 time windows, evolution of the L^2 relative error accross the time, final time $T = 20$



Sometimes instability



Speed up



8
7
6
5
4
3
2
1
Speed up
2
4
6
8
10
12
14
16
Number of processes
Optimal speed up
Speed up (220 cells) $\Delta t_{\text{coarse}} = 20\ \delta t_{\text{fine}}$
Speed up (110 cells) $\Delta t_{\text{coarse}} = 20\ \delta t_{\text{fine}}$

Conclusions and perspectives

- Parareal algorithm for separated phases test case
- Coarsen spatial discretisation also, keep coarse and fine solvers at constant CFL and use high order interpolation (Thesis T. Lunet)
- Parareal algorithm for boiling flows

M. J. Gander, I. Kulchytska-Ruchka, I. Niyonzima, and S. Schöps, A New Parareal Algorithm for Problems with Discontinuous Sources