

A Computational Fluid Dynamics (CFD) Benchmark Study with an Analysis of Richardson Extrapolation in the Presence of a Singularity

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Goals

French Thermal Engineering Society (SFT), Benchmark workgroup:

- Propose a **reference solution** for a 3D **mixed convection** flow;
- Systematic use of **Richardson extrapolation** for solution verification.

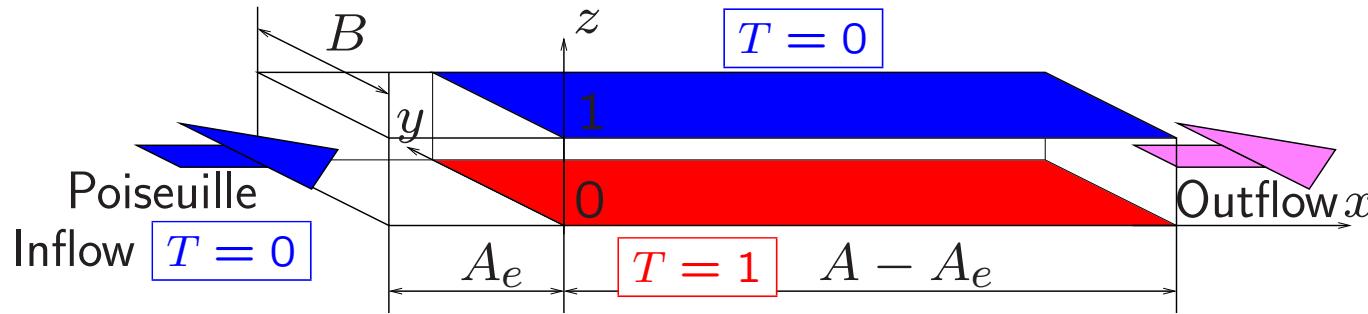
Timeline:

- Call for contributions [2006, International Journal of Thermal Sciences];
- Publications [2011, Numerical Heat Transfer].

Outline

1. The benchmark problem and contributors' solvers;
2. Richardson Extrapolation;
3. Results;
4. Analysis of the results: Singularity;
5. Analysis of the results: Richardson extrapolation behavior;
6. Conclusion.

3D mixed convection flow: Poiseuille-Rayleigh-Bénard instability



Incompressible Navier-Stokes + Boussinesq

Mass: $\nabla \cdot \mathbf{u} = 0$

Momentum: $\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \Delta \mathbf{u} + \frac{Ra}{Pr Re^2} T \mathbf{i}_z$

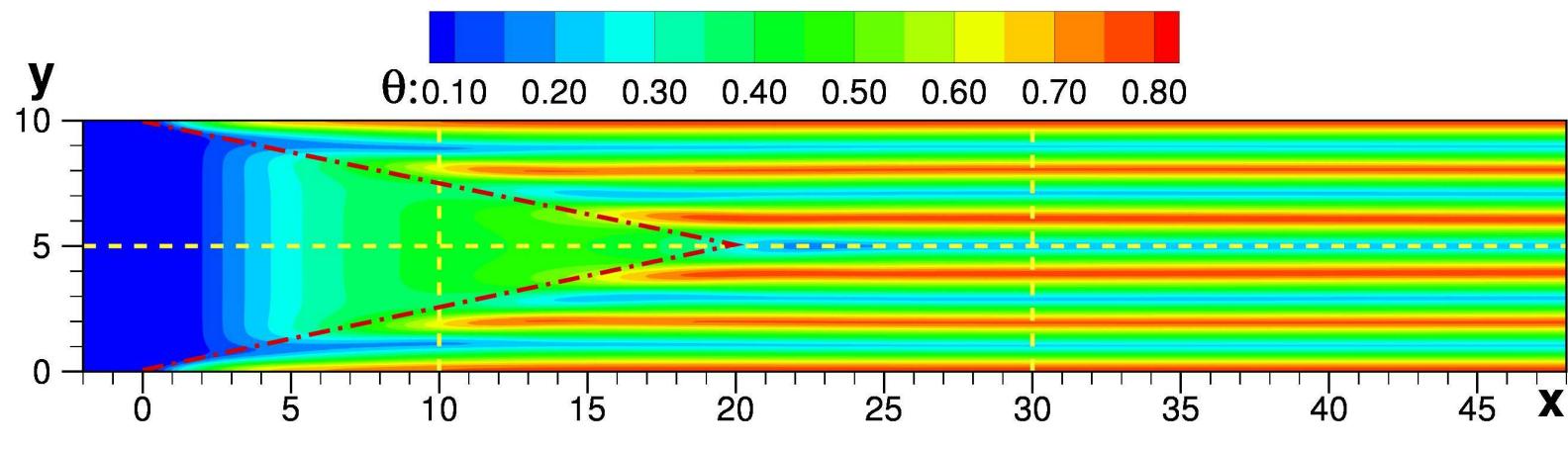
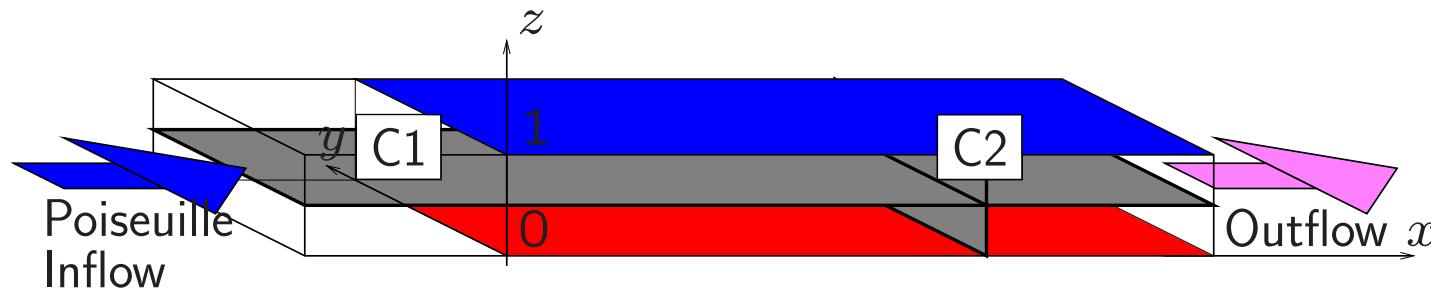
Energy: $\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{Pr Re} \Delta T$

Non dimensional parameters

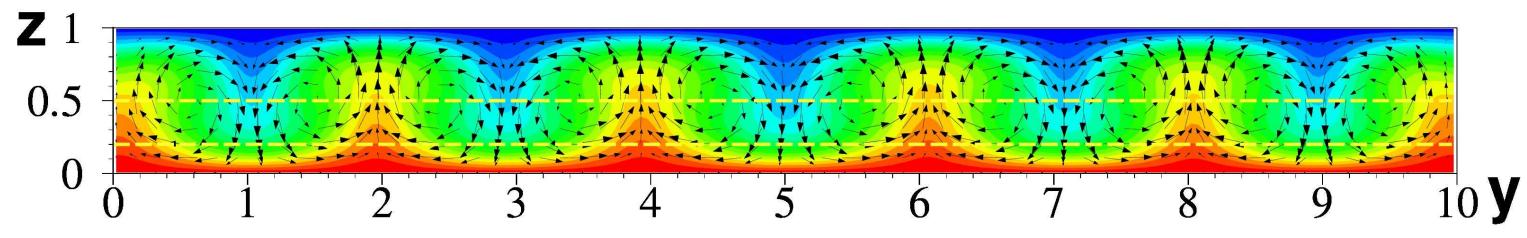
Geometry: $A = 50$ $A_e = 2$ $B = 10$

Physics: $Pr = 0.7$ $Re = 50$ $Ra = 5000$

Poiseuille-Rayleigh-Bénard flow



$$C_1 \quad z = \frac{1}{2}$$



$$C_2 \quad x = 30$$

Solution method

| | FD1 | FE2 | FV3 | FE4 |
|----------------------------------|------------------------------|-----------------------------|-----------------------------|-----------------------------|
| Contributor | X. Nicolas | M. Medale | S. Glockner | S. Gounand |
| Spatial disc. | Finite Difference | Finite Element | Finite Volume | Finite Element |
| Consistency order α° | u, T 2 | 3 | 2 | 3 |
| p | 2 | 2 | 2 | 2 |
| Finest mesh | $1200 \times 400 \times 120$ | $1351 \times 271 \times 91$ | $1351 \times 361 \times 91$ | $1001 \times 201 \times 81$ |
| Solver | | Projection method | | |

Quantities of Interest (QOI):

| | | |
|---------------|------------------------------------|---|
| Integrals | Kinetic energy | $2E_c = \frac{1}{ \Omega } \int_{\Omega} \mathbf{u} ^2 d\Omega$ |
| | Mean Pressure difference | $\Delta P_{io} = \frac{1}{ S_o } \int_{S_o} P dS_o - \frac{1}{ S_i } \int_{S_i} P dS_i$ |
| | Mean temperature | $T_m = \frac{1}{ \Omega } \int_{\Omega} T d\Omega$ |
| Boundary flux | thermal, momentum | |
| Local extrema | primal variables \mathbf{u}_i, T | flux (Nusselt number) |

Richardson Extrapolation (1911)

Taylor expansion for the QOI f (regular enough) in the **discretization parameter** h :

$$f_h = f_{\text{exact}} + C_\alpha h^\alpha + O(h^{\alpha+1})$$

Asymptotic range:

$$C_\alpha h_i^\alpha \gg O(h_i^{\alpha+1})$$

Uniform space-time refinement:

3 grids: $h_1, h_2, h_3 \Rightarrow$ 3 solutions: f_1, f_2, f_3

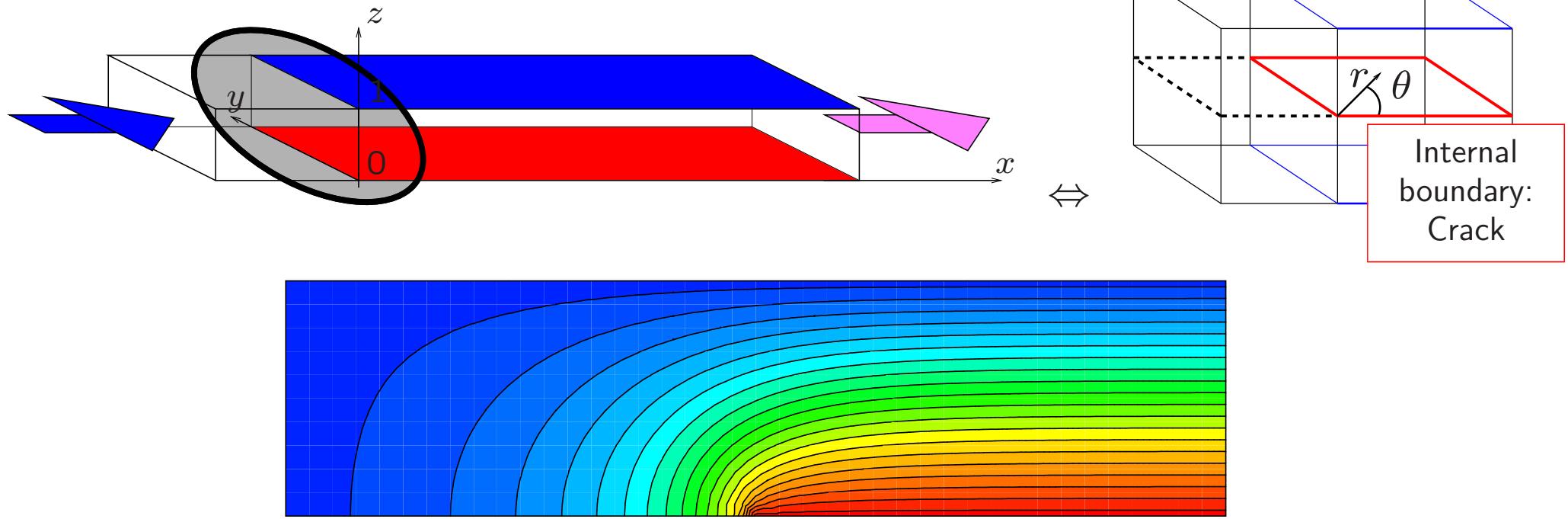
Then:

| 3 unknowns | 3 informations |
|---|-----------------------------|
| $\tilde{\alpha} = \frac{\log((f_{h_1} - f_{h_2})/(f_{h_2} - f_{h_3}))}{\log(h_1/h_2)}$ | Convergence order |
| if $\frac{h_1}{h_2} = \frac{h_2}{h_3}$: $\tilde{C}_\alpha = \frac{f_{h_2} - f_{h_3}}{h_2^{\tilde{\alpha}} - h_3^{\tilde{\alpha}}}$ | Error estimate (not robust) |
| $f^{\text{extrapolated}} = f_{h_3} - \tilde{C}_\alpha h_3^{\tilde{\alpha}}$ | Enhanced precision |

Results

| | | FD1 | FE2 | FV3 | FE4 |
|---------------------------------------|--------|------------|------------|-------------|------------|
| Contributor | | X. Nicolas | M. Medale | S. Glockner | S. Gounand |
| Consistency | u, T | 2 | 3 | 2 | 3 |
| order α° | p | 2 | 2 | 2 | 2 |
| $2E_c^{\text{fine grid}}$ | | 1.292479 | 1.292452 | 1.292355 | 1.292461 |
| $2E_c^{\text{extrapolated}}$ | | 1.292446 | 1.292452 | 1.292455 | 1.292467 |
| α_{E_c} | | 2.22 | 2.92 | 2.00 | -1.92 |
| $\Delta P_{io}^{\text{fine grid}}$ | | 14.41210 | 14.40784 | 14.40235 | 14.40694 |
| $\Delta P_{io}^{\text{extrapolated}}$ | | 14.40647 | 14.40649 | 14.40678 | 14.40658 |
| $\alpha_{\Delta P_{io}}$ | | 2.03 | 1.99 | 2.00 | 0.83 |
| $T_m^{\text{fine grid}}$ | | 0.448490 | 0.448625 | 0.448725 | 0.448659 |
| $T_m^{\text{extrapolated}}$ | | 0.448594 | 0.448604 | 0.448606 | 0.448613 |
| α_{T_m} | | 1.19 | 1.18 | 1.02 | 1.18 |

Singularity: stiff transition in the boundary conditions



Singular solution behavior : $T_{\text{exact}} \approx r^{\frac{1}{2}} \sin 2\theta$

A priori error estimation: $T_h = T_{\text{exact}} + Ch^{\min(s, \alpha^\circ)}$ [1973, Strang & Fix]

In our case: $s = 1$ and $\alpha^\circ = 2$ or 3

Results revisited

| | | FD1 | FE2 | FV3 | FE4 |
|---------------------------------------|-----|------------|------------|-------------|------------|
| Contributor | | X. Nicolas | M. Medale | S. Glockner | S. Gounand |
| Consistency \mathbf{u}, T | | 2 | 3 | 2 | 3 |
| order α° | p | 2 | 2 | 2 | 2 |
| $2E_c^{\text{fine grid}}$ | | 1.292479 | 1.292452 | 1.292355 | 1.292461 |
| $2E_c^{\text{extrapolated}}$ | | 1.292446 | 1.292452 | 1.292455 | 1.292467 |
| α_{E_c} | | 2.22 | 2.92 | 2.00 | -1.92 |
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| α_{T_m} | | 1.19 | 1.18 | 1.02 | 1.18 |

$\alpha \neq 1 \Rightarrow \text{not in the asymptotic range!}$

Model function

In practice: $h \neq 0$

Definition: $\underline{g_h = g_{\text{exact}} + C_s h^s + C_{\alpha^\circ} h^{\alpha^\circ}}$

Scaling: $(h_1, h_2, h_3) = (1, 1/\tau, 1/\tau^2)$ and $g_{\text{exact}} = 1$

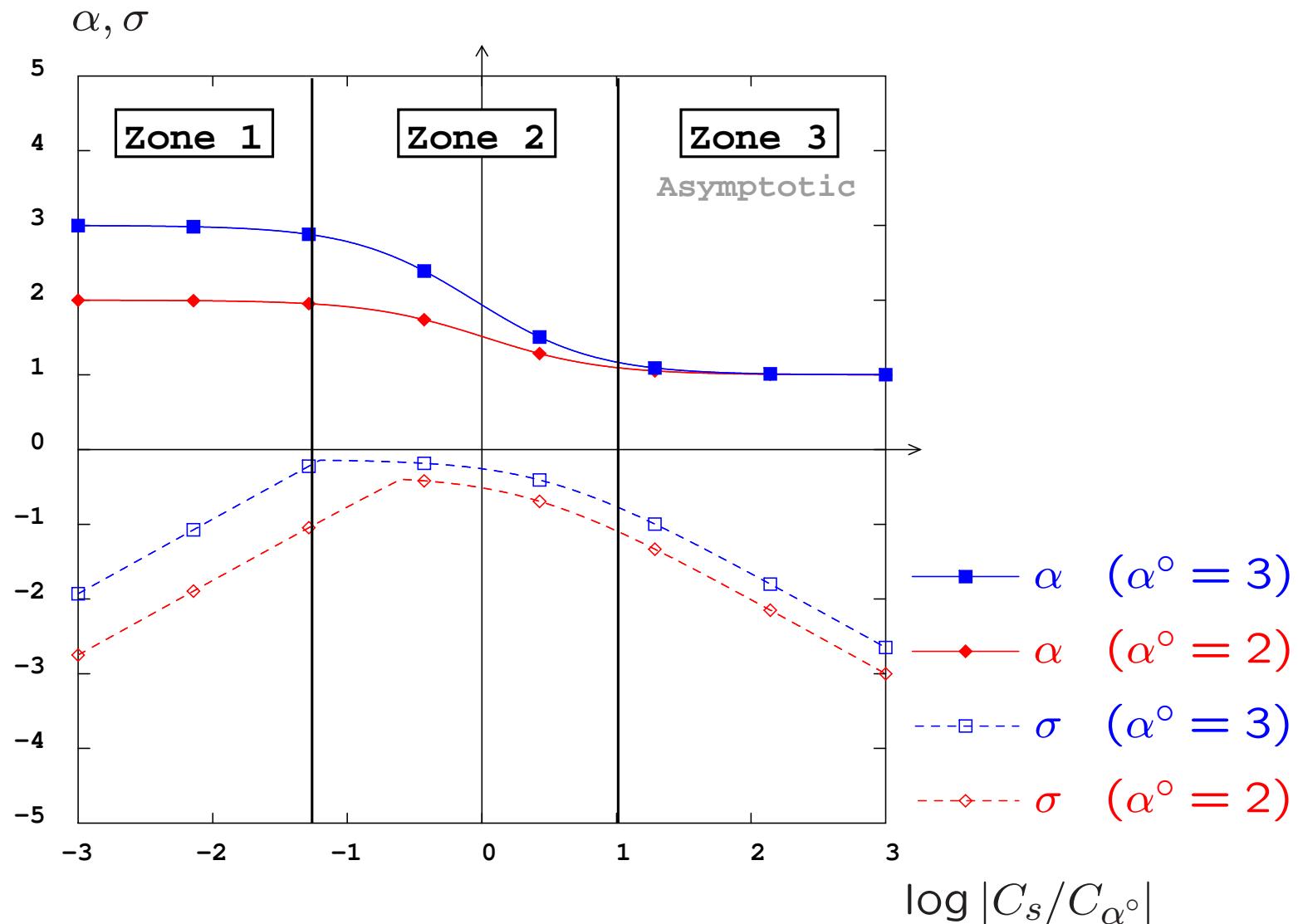
Fixed parameters: $\tau = 2, C_{\alpha^\circ} = 10^{-4}, s = 1$

Variable parameters: $\rho = C_s/C_{\alpha^\circ}, \alpha^\circ = 2 \text{ or } 3$

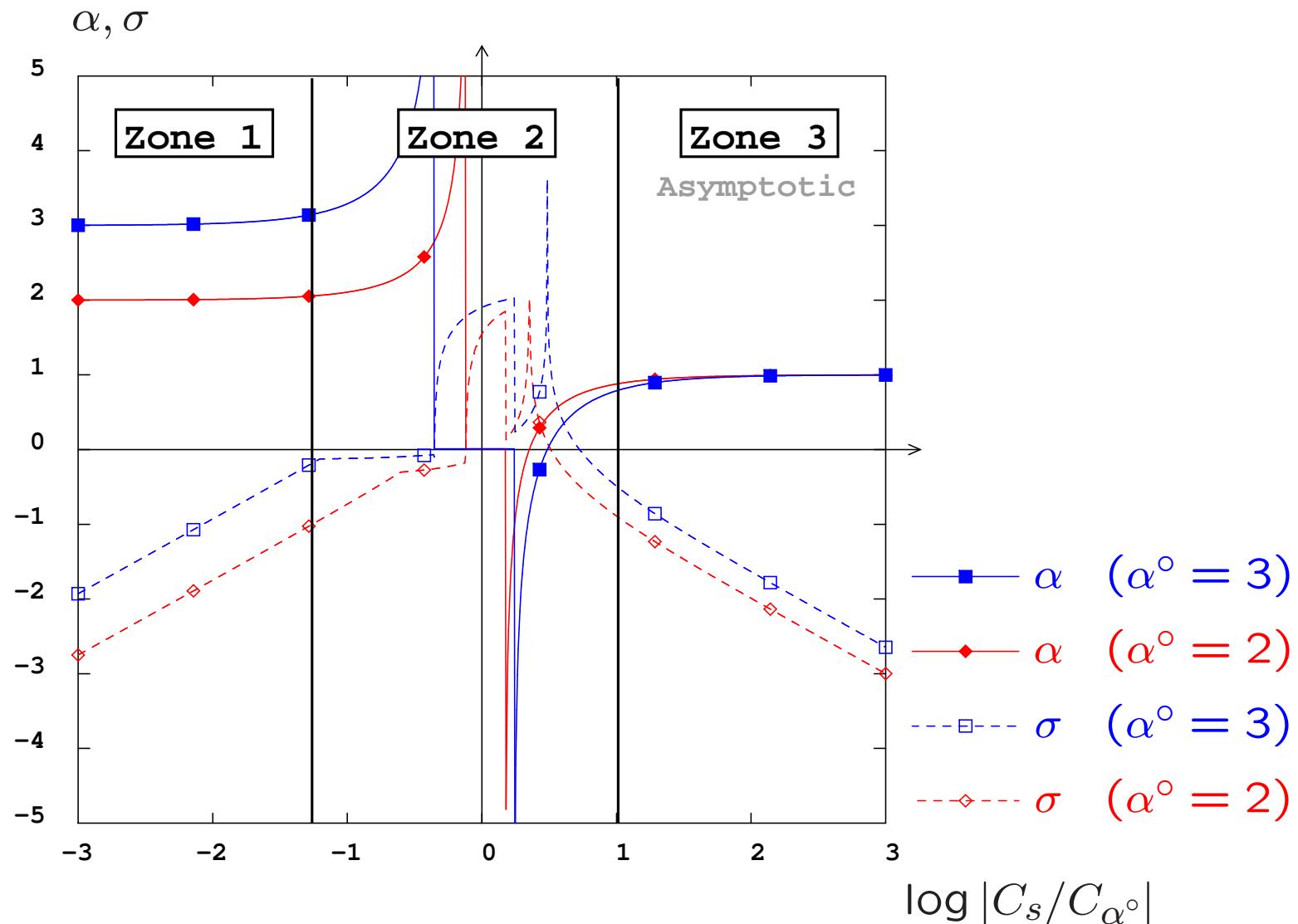
Apply Richardson Extrapolation Formulae (slide 7) on g_h

QOI: Convergence order $\boxed{\alpha}$ and Richardson efficiency ratio $\boxed{\sigma} = \log \frac{|g^{\text{extrapolated}} - g_{\text{exact}}|}{\max(|C_{\alpha^\circ} h_3^{\alpha^\circ}|, |C_s h_3^s|)}$

Richardson extrapolation on g_h : $\rho = C_s/C_{\alpha^\circ} > 0$



Richardson extrapolation on g_h : $\rho = C_s/C_{\alpha^\circ} < 0$



Results rerevisited

| | | FD1 | FE2 | FV3 | FE4 |
|---------------------------------------|--------|------------|------------|-------------|------------|
| Contributor | | X. Nicolas | M. Medale | S. Glockner | S. Gounand |
| Consistency order α° | u, T | 2 | 3 | 2 | 3 |
| | p | 2 | 2 | 2 | 2 |
| $2E_c^{\text{fine grid}}$ | | 1.292479 | 1.292452 | 1.292355 | 1.292461 |
| $2E_c^{\text{extrapolated}}$ | | 1.292446 | 1.292452 | 1.292455 | 1.292467 |
| α_{E_c} | | 2.22 | 2.92 | 2.00 | -1.92 |
| $\Delta P_{io}^{\text{fine grid}}$ | | 14.41210 | 14.40784 | 14.40235 | 14.40694 |
| $\Delta P_{io}^{\text{extrapolated}}$ | | 14.40647 | 14.40649 | 14.40678 | 14.40658 |
| $\alpha_{\Delta P_{io}}$ | | 2.03 | 1.99 | 2.00 | 0.83 |
| $T_m^{\text{fine grid}}$ | | 0.448490 | 0.448625 | 0.448725 | 0.448659 |
| $T_m^{\text{extrapolated}}$ | | 0.448594 | 0.448604 | 0.448606 | 0.448613 |
| α_{T_m} | | 1.19 | 1.18 | 1.02 | 1.18 |

Guideline: it seems safe to keep $f^{\text{extrapolated}}$ when α is near s or α° .

Conclusion

- A reference solution for 3D steady mixed convection flow: **4 or 5 significant digits**;

Nicolas, X., Medale, M., Glockner, S., and Gounand, S. (2011c). Benchmark solution for a three-dimensional mixed-convection flow, part 1: Reference solutions. *Numerical Heat Transfer, Part B: Fundamentals*, 60(5):325–345

- An analysis of Richardson extrapolation and its **practical implications**;

Nicolas, X., Gounand, S., Medale, M., and Glockner, S. (2011a). Benchmark solution for a three-dimensional mixed-convection flow, part 2: Analysis of richardson extrapolation in the presence of a singularity. *Numerical Heat Transfer, Part B: Fundamentals*, 60(5):346–369

- SFT Technical Report.

Nicolas, X., Medale, M., Glockner, S., and Gounand, S. (2011b). Benchmark solution for a three-dimensional mixed-convection flow—detailed technical report. Technical report. http://www.sft.asso.fr/Local/sft/dir/user-3775/documents/DocumentsDivers/SFT_Report_benchmark_PRB_2011.pdf

The end

Thank you for your attention.

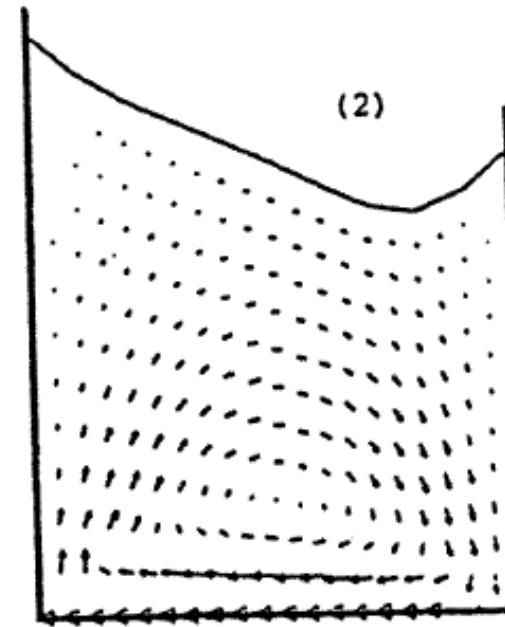
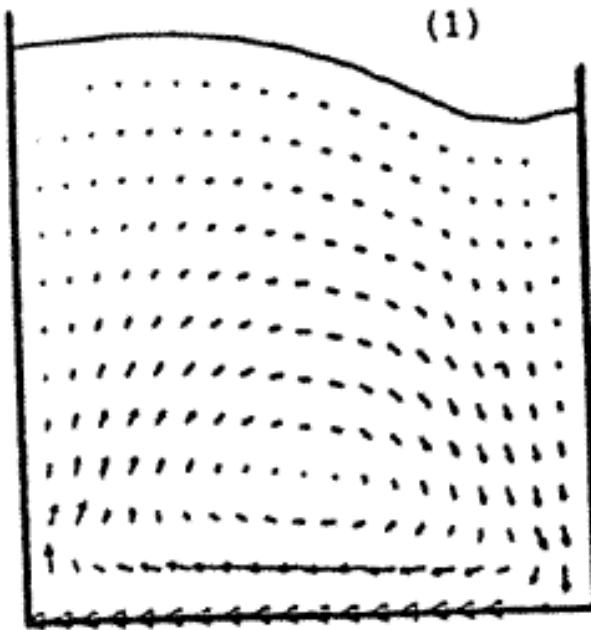
Appendix : Perspectives (I)

- Verify that the analysis done for the model function translates to the Benchmark computations
⇒ fine meshes;
- Call for participations [Medale and Nicolas, 2006]: unsteady case with a difficult free-exit boundary condition;

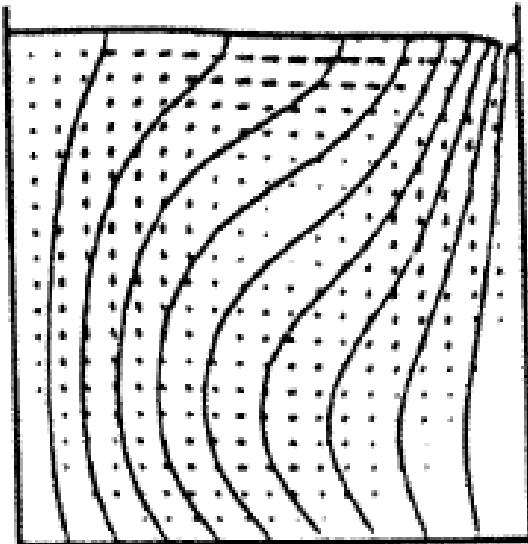
$$Pr = 7 \quad Re = 0.1 \quad Ra = 2500$$

- Free surface benchmark problem

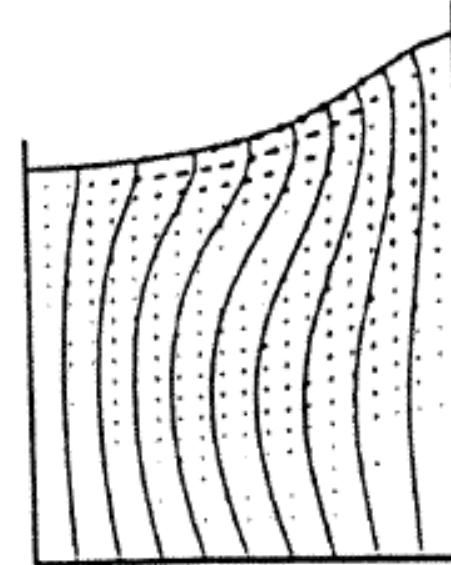
Appendix : Free surface benchmark problem (II)



Steady flow with surface tension [Cuvelier and Schulkes, 1990]

Appendix : Free surface benchmark problem (III)

(b)



(c)

Steady flow with Marangoni effect [Cuvelier and Schulkes, 1990]

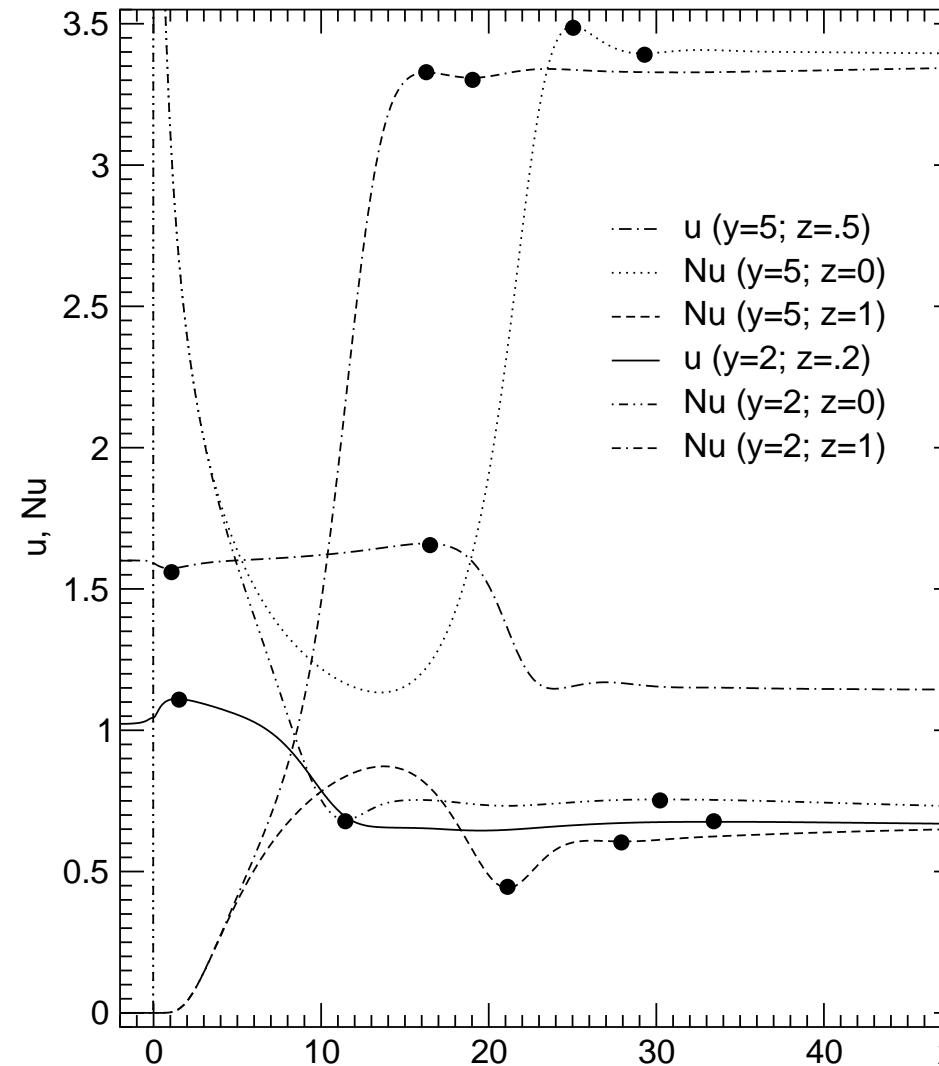
Appendix : More on the solution method (IV)

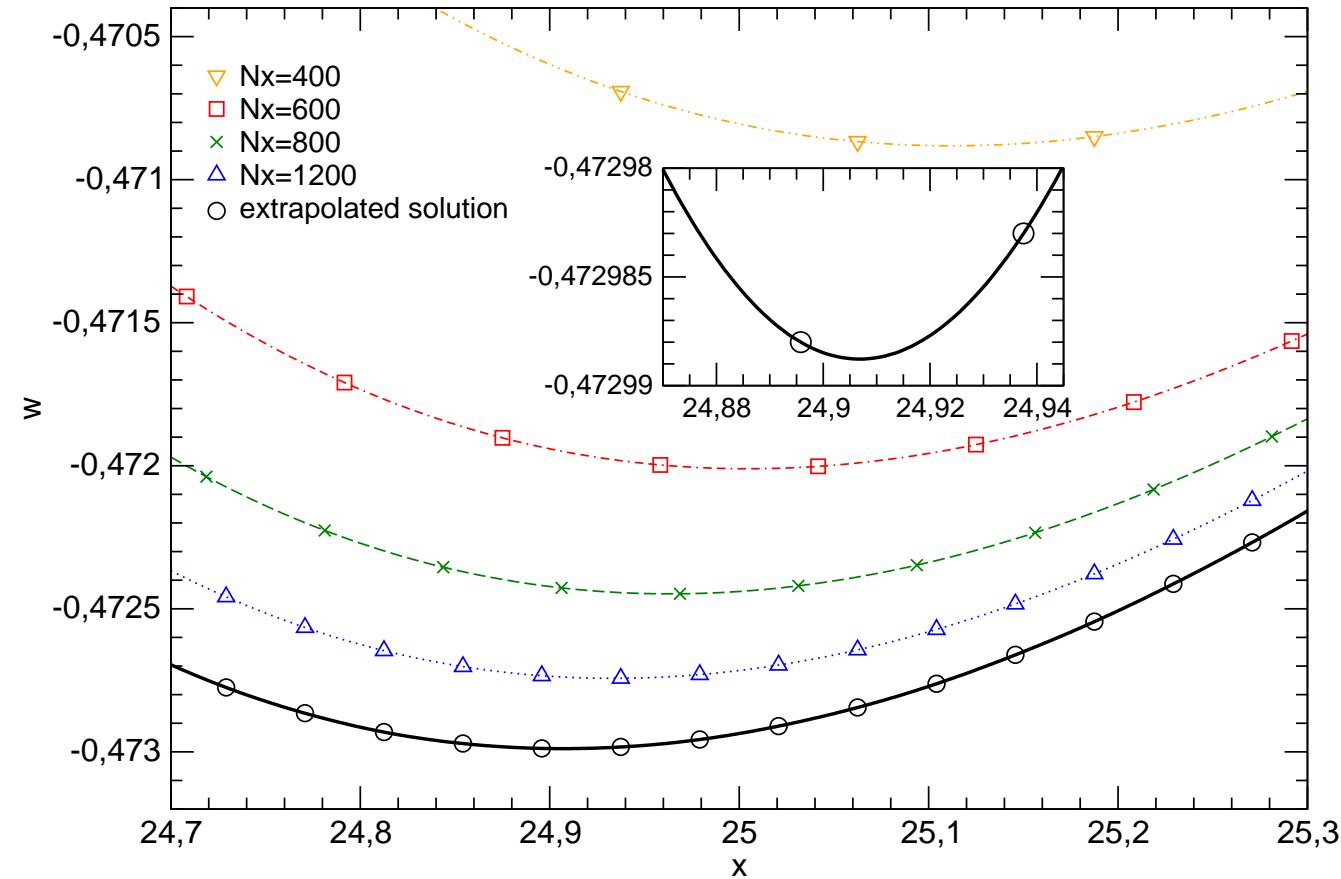
4 different solution method and codes :

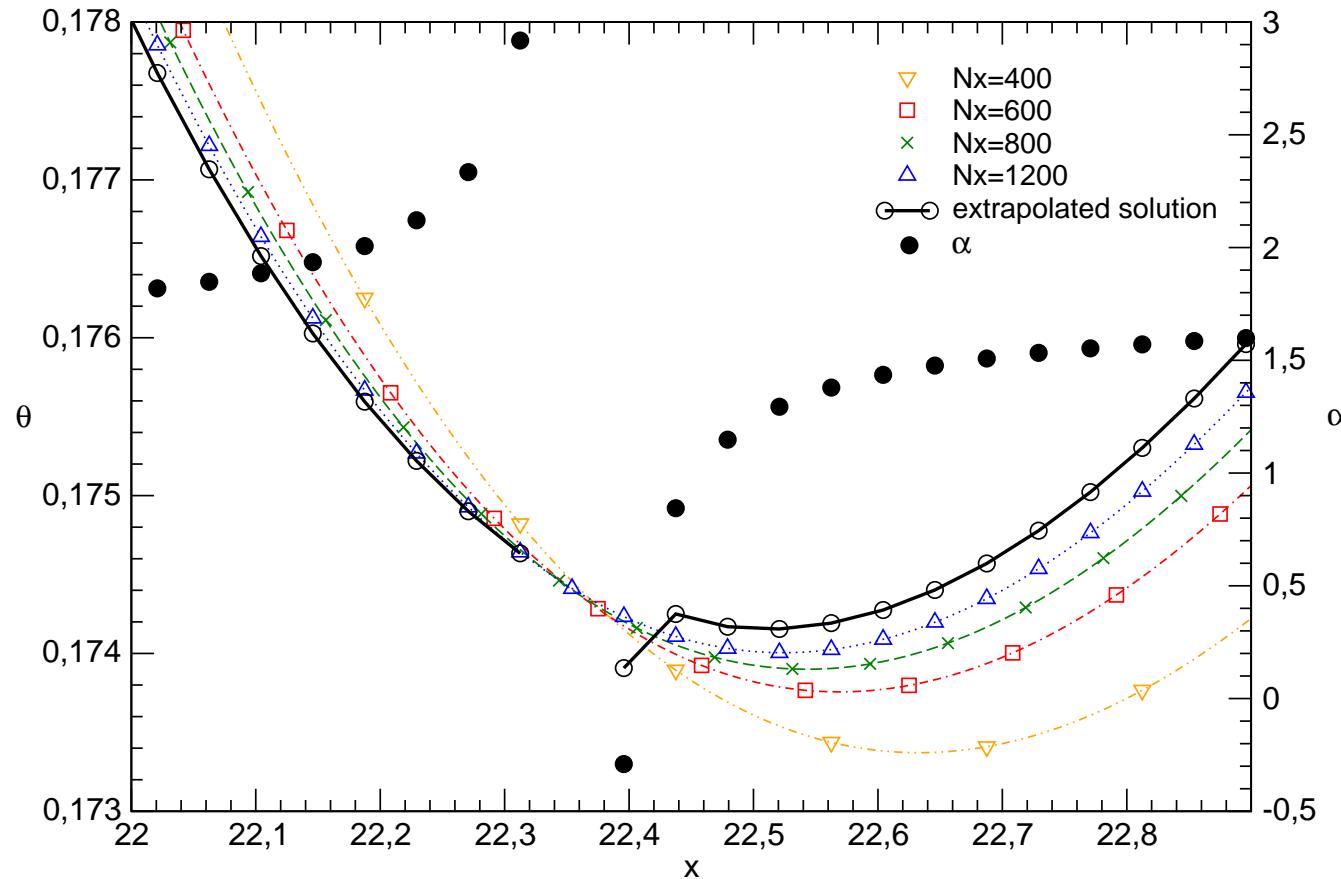
- FD1** Centered Finite Difference, vectorized, ADI, tridiagonal matrices, continuous projection method (Goda);
- FE2** Q2/Q1 finite elements, distributed parallelism, domain decomposition (PETSc), continuous projection method (Guermond) ;
- FV3** Thétis, nodal finite volumes, face-centered velocity, QUICK upwinding on temperature, distributed parallelism (Hypre), continuous projection method (Timmermans) ;
- FE4** Cast3m, Q2/P1nc finite elements, shared-memory parallelism, AGMG (Notay), algebraic projection method (Quarteroni).

Appendix : Contributors' parameters (V)

| Contributor | $N_x \times N_y \times N_z$ [symmetry] | Δt | User time [computer type (organism/lab)] | Consistency orders α° |
|--------------------------|---|------------|--|--|
| MSME, FD1 | 400 × 134 × 40 | 0.01 | 36 min on 1 processor | 2 for $\theta, u, v, w;$ 2 for p |
| | 600 × 200 × 60 | 0.01 | 2 h 20 on 1 processor | |
| | 800 × 268 × 80 | 0.002 | 25 h on 1 processor | |
| | 1200 × 400 × 120 | 0.002 | 100 h on 1 processor | |
| | [no] | | [NEC SX5 (IDRIS)] | |
| IUSTI, FE2 | 601 × 121 × 41 | 0.01 | 19 min on 60 cores | 3 for $\theta, u, v, w;$ 2 for p |
| | 901 × 181 × 61 | 0.01 | 1 h 40 on 150 cores | |
| | 1351 × 271 × 91 | 0.005 | 43 h 15 on 225 cores | |
| | [yes] | | [IBM SP6 (IDRIS)] | |
| I2M Institute, FV3 | 601 × 161 × 41 | 0.1 | 8 h on 152 cores | 2 for $\theta, u, v, w;$ 2 for p |
| | 901 × 241 × 61 | 0.1 | 12 h on 152 cores | |
| | 1351 × 361 × 91 | 0.1 | 56 h on 152 cores | |
| | [yes] | | [ALTIX ICE 8200 (I2M Inst.)] | |
| CEA, FE4 | 601 × 121 × 49 | 0.5 | 200 h on 8 cores | 3 for $\theta, u, v, w;$ 2 for p |
| | 751 × 151 × 61 | 0.5 | 400 h on 8 cores | |
| | 801 × 161 × 65 | 0.5 | 450 h on 8 cores | |
| | 1001 × 201 × 81 | 0.5 | 1600 h on 8 cores | |
| | [yes] | | [PC 8 cores (CEA)] | |

Appendix : Example of profiles (VI)

Appendix : Richardson Extrapolation on profiles (VII)

Appendix : Richardson Extrapolation on intersecting profiles (VIII)

Appendix : Remarks on the usage of Richardson Extrapolation (IX)

Some authors (including Richardson himself!) choose $\alpha = \alpha^\circ$.

Advantages:

- only two grids needed;
- no problem with intersecting profiles.

Drawback:

- no verification of the convergence order (extrapolated value possibly unprecise).

Appendix : Cast3m (X)

Main features:

- General purpose Finite Element code developed at CEA (French Alternative Energies and Atomic Energy Commission);
- Simple user-level scripting language (Matlab-like);
- Can be used in a white-box fashion (source);
- Integrated pre- and post-processing;
- Online documentation (french, english);
- Free for research use or teaching.

<http://www-cast3m.cea.fr/>

Appendix : Algebraic Projection Method (XI)

Continuous Incompressible Navier-Stokes

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = \mathbf{f} \\ \nabla \cdot \mathbf{u} = g \end{cases}$$

Discrete Navier-Stokes

$$\begin{cases} \mathbf{A}_u \mathbf{u} + \mathbf{G}p = \mathbf{f} \\ \mathbf{D}\mathbf{u} = g \end{cases}$$

Linearization and an incremental method (Newton)

$$\begin{pmatrix} \mathbf{A}' & \mathbf{G} \\ \mathbf{D} & 0 \end{pmatrix} \begin{pmatrix} \delta \mathbf{u} \\ \delta p \end{pmatrix} = \begin{pmatrix} \mathbf{f} - \mathbf{A}_{u_i} \mathbf{u}_i - \mathbf{G}p_i \\ g - \mathbf{D}\mathbf{u}_i \end{pmatrix} = \begin{pmatrix} \delta \mathbf{f} \\ \delta g \end{pmatrix}$$

Appendix : Algebraic Projection (XII)

Block LU factorization (A invertible)

$$\begin{pmatrix} A & G \\ D & 0 \end{pmatrix} = \begin{pmatrix} A & 0 \\ D & -DA^{-1}G \end{pmatrix} \begin{pmatrix} I & A^{-1}G \\ 0 & I \end{pmatrix}$$

Approximation : $H \approx A^{-1}$

LU factorization of an approximate tangent matrix

$$\begin{pmatrix} A & AHG \\ D & 0 \end{pmatrix} = \begin{pmatrix} A & 0 \\ D & -DHG \end{pmatrix} \begin{pmatrix} I & HG \\ 0 & I \end{pmatrix}$$

Appendix : Algebraic Projection (XIII)

Step by step solution (\equiv splitting method)

$$\left(\begin{array}{cc} \boxed{A}_1 & 0 \\ D & \boxed{-DHG}_2 \end{array} \right) \underbrace{\left(\begin{array}{c} \boxed{I}_4 \\ 0 \\ \boxed{HG} \\ \boxed{I}_3 \end{array} \right)}_{\left(\begin{array}{c} \delta \tilde{u} \\ \delta \tilde{p} \end{array} \right)} = \left(\begin{array}{c} \delta f \\ \delta g \end{array} \right)$$

Etape

| | | |
|---|---|--|
| 1 | $A \delta \tilde{u} = \delta f$ | Force balance |
| 2 | $-DHG \delta \tilde{p} = \delta g - D \delta \tilde{u}$ | Lagrange multiplier computation |
| 3 | $\delta p = \delta \tilde{p}$ | (Discrete pressure Laplacian) |
| 4 | $\delta u = \delta \tilde{u} - HG \delta p$ | Constraint satisfaction (mass balance) |

Appendix : Algebraic Projection (XIV)

Advantages:

- Efficient method for solving the 3D unsteady incompressible Navier-Stokes equations;
- Exact constraint satisfaction (mass balance).

Drawbacks:

- Slow convergence when δt is large (loss of efficiency when $H \not\approx A^{-1}$).

Bibliography

[Strang and Fix, 1988] Strang, W. and Fix, G. (1988). *An Analysis of the Finite Element Method*. Wellesley-Cambridge Press, 2nd edition. chapter 8.

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[Cuvelier and Schulkes, 1990] Cuvelier, C. and Schulkes, R. (1990). Some numerical methods for the computation of capillary free boundaries governed by the Navier-Stokes equation. *SIAM Review*, 32(3):355–423.