Numerical Solutions of Partial Diffirential Equations

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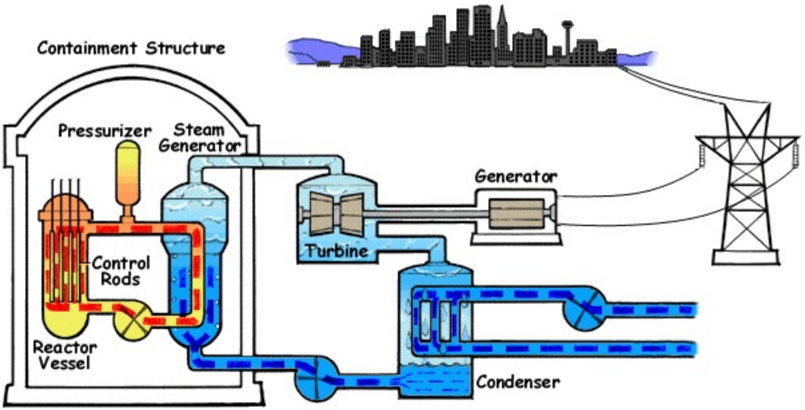

Figure: Pressurized Water Reactor

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Finite volume discretisation

$$\frac{\partial U}{\partial t} + \nabla . (\mathcal{F}(U)) = 0 \tag{1}$$

Integrating (1) over C_i

$$\frac{\partial}{\partial t}\left(\int_{C_i} U(x,t)\,\mathrm{d}\vec{x}\right) + \sum_{j\in N(i)} \int_{\partial C_{ij}} \mathcal{F}(U).\vec{n_{ij}}\,\mathrm{d}s = 0 \tag{2}$$

Set $U_i(t) = \frac{1}{v_i}\int_{C_i} U(x,t)dx$, we have

$$\frac{\partial}{\partial t}\left(\int_{C_i} U(x,t)\,\mathrm{d}\vec{x}\right) \cong v_i \frac{\partial U_i(t)}{\partial t} \cong v_i \frac{U_i^{n+1} - U_i^n}{\Delta t}$$

Finite volume discretisation

We obtain the numerical scheme

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \sum_{j \in N(i)} \frac{1}{v_i} \overrightarrow{\Phi}_{ij} s_{ij} = 0$$

with the numerical flux: $\overrightarrow{\Phi}_{ij} = \frac{1}{s_{ij}} \int_{\partial C_{ij}} \mathcal{F}(U).\vec{n_{ij}} \, \mathrm{d}s$

Usually, the numerical flux $\vec{\Phi}_{ij}$ is defined by solving exactly/ approximately a Riemann problem:

$$\begin{cases} \frac{\partial U}{\partial t} + \nabla . (\mathcal{F}(U)) = 0 \\ U(x,t) = \begin{cases} U_i & \text{if } x \in C_i \\ U_j & \text{if } x \in C_j \end{cases} \end{cases} \quad \text{or} \quad \begin{cases} \frac{\partial U}{\partial t} + \frac{\partial \vec{F}_{\vec{n}}}{\partial \vec{n}} \frac{\partial U}{\partial \vec{n}} = 0 \\ U(x,t) = \begin{cases} U_i & \text{if } \vec{x}.\vec{n} < 0 \\ U_j & \text{if } \vec{x}.\vec{n} > 0 \end{cases} \end{cases}$$

Finite volume discretisation

And we have the numerical flux $\vec{\Phi}_{ij}$:

$$\overrightarrow{\Phi}_{ij} = \frac{F(U_i) + F(U_j)}{2}.\vec{n}_{ij} - \mathcal{D}(U_i, U_j)\frac{U_j - U_i}{2}$$

Various choices for $\mathcal{D}(U_i, U_j)$:

- $\mathcal{D} = 0$: centered scheme.
- $\mathcal{D} = |A_{Roe,\vec{n}_{ij}}|$: upwind scheme.
- $\mathcal{D} = \rho(A)\mathbf{I}$: Rusanov scheme etc ...

Roe scheme

Replace the exact nonlinear Riemann problem by a approximate problem linearized between cells i and j

$$\frac{\partial U}{\partial t} + A(U_i, U_j, \vec{n}_{ij})\frac{\partial U}{\partial \vec{n}_{ij}} = 0$$

$A_{Roe,\vec{n}_{ij}}(U_i, U_j) = A(U_i, U_j, \vec{n}_{ij})$ satisfies 3 conditions:

1. $A_{Roe,\vec{n}_{ij}}$ is diagonalizable
2. Consistency: $A_{Roe,\vec{n}_{ij}}(U_i, U_i) = \nabla F_{\vec{n}}(U_i)$
3. Conservation: $(F(U_i) - F(U_j)).\vec{n}_{ij} = A_{Roe,\vec{n}_{ij}}(U_i - U_j)$

Roe scheme

The Roe's numerical flux:

$$\begin{aligned}\overrightarrow{\Phi}_{ij} &= \frac{F(U_i)+F(U_j)}{2}.\vec{n}_{ij} - |A_{Roe,\vec{n}_{ij}}|\frac{U_j - U_i}{2} \\ &= F(U_i)\overrightarrow{n}_{ij} + A^-_{Roe,\vec{n}_{ij}}(U_j - U_i) \\ &= F(U_j)\overrightarrow{n}_{ij} - A^+_{Roe,\vec{n}_{ij}}(U_j - U_i)\end{aligned}$$

with $|A|$ the absolute value of A, $A^+ = \frac{A+|A|}{2}$, $A^- = \frac{A-|A|}{2}$
The final scheme:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \sum_{j\in N(i)} \frac{s_{ij}}{v_i} A^-_{Roe,\vec{n}_{ij}}(U_j - U_i) = 0$$

The Single-phase Flows

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla . \overrightarrow{q} = 0 \\ \frac{\partial \overrightarrow{q}}{\partial t} + \nabla . \left(\overrightarrow{q} \otimes \frac{\overrightarrow{q}}{\rho} + p\mathbf{I} \right) - \nu \Delta \left(\frac{\overrightarrow{q}}{\rho} \right) = 0 \\ \frac{\partial (\rho E)}{\partial t} + \nabla . \left[(\rho E + p) \frac{\overrightarrow{q}}{\rho} \right] - \lambda \Delta T = 0 \end{cases}$$

Eq of state: $p = (\gamma - 1) e \rho$.

- ρ : density
- $\overrightarrow{q}$: momentum
- p : pressure
- e : internal energy
- E : total energy
- T : temperature
- ν : viscosity
- λ : conductivity

Numerical Schemes

$$\frac{\partial U}{\partial t} + \nabla . (\mathcal{F}^{conv}(U)) + \nabla . \left(\mathcal{F}^{diff}(U)\right) = 0 \qquad (3)$$

U the vector of unknown physical quantities
$\mathcal{F}^{conv}(U)$ the flux of convection, $\mathcal{F}^{diff}(U)$ the flux of diffusion
Finite volume formulation

$$\int_{C_i} \frac{\partial U}{\partial t} \mathrm{d}\vec{x} + \sum_{j \in N(i)} \int_{\partial C_{ij}} \left(\mathcal{F}^{conv}(U).\vec{n_{ij}} + \mathcal{F}^{diff}(U).\vec{n_{ij}}\right) \mathrm{d}s = 0 \quad (4)$$

Set $U_i(t) = \frac{1}{v_i} \int_{C_i} U(x,t)dx$ and $U_i^n = U_i(n\Delta t)$, we have:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \sum_{j \in N(i)} \frac{s_{ij}}{v_i} (\overrightarrow{\Phi^{conv}}_{ij} + \overrightarrow{\Phi}_{ij}^{diff}) = 0 \qquad (5)$$

$$(6)$$

Use Roe's scheme of the numerical flux of convection $\overrightarrow{\Phi}_{ij}^{conv}$:

$$\begin{aligned} \overrightarrow{\Phi}_{ij}^{conv} &= \frac{\mathcal{F}^{conv}(U_i) + \mathcal{F}^{conv}(U_j)}{2}.\vec{n}_{ij} + \mathcal{D}\frac{U_j - U_i}{2} & (7) \\ &= \mathcal{F}^{conv}(U_i)\overrightarrow{n}_{ij} + A^-(U_i, U_j)(U_j - U_i). & (8) \end{aligned}$$

with $A^- = \frac{A-\mathcal{D}}{2}$ and A is a Roe's matrix.

For the numerical flux of diffusion $\overrightarrow{\Phi}_{ij}^{diff}$ on structured meshes:

$$\overrightarrow{\Phi}_{ij}^{diff} = D(U_i, U_j)(U_j - U_i) \qquad (9)$$

Explicit system

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \sum_{j \in N(i)} \frac{s_{ij}}{v_i}\{(A^- + D)(U^n)\}(U_j^n - U_i^n) = 0 \qquad (10)$$

Implicit scheme

Implicit non linear system

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \sum_{j \in N(i)} \frac{s_{ij}}{v_i} \{(A^- + D)(U^{n+1})\}(U_j^{n+1} - U_i^{n+1}) = 0 \tag{11}$$

We have the equation: $f(U) = 0$, with:

$$f(U)|_i = \frac{U_i - U_i^n}{\Delta t} + \sum_{j \in N(i)} \frac{s_{ij}}{v_i} \{(A^- + D)(U_i, U_j)\}(U_j - U_i)$$

We solve with the Newton iterative algorithm:

$$f'(U^k)(U^{k+1} - U^k) + f(U^k) = 0$$

Newton scheme

Solve several linear systems to obtain the required solutions:

$$\frac{\delta U_i^{k+1}}{\Delta t} + \sum_{j\in N(i)} \frac{s_{ij}}{v_i}\left[(A^- + D)(U_i^k, U_j^k)\right]\left(\delta U_j^{k+1} - \delta U_i^{k+1}\right)$$
$$= -\frac{U_i^k - U_i^n}{\Delta t} - \sum_{j\in N(i)} \frac{s_{ij}}{v_i}\left[(A^- + D)(U_i^k, U_j^k)\right](U_j^k - U_i^k),$$

where $\delta U_i^{k+1} = U_i^{k+1} - U_i^k$.
Each Newton iteration requires the numerical solution of the following linear system:

$$\mathcal{A}(\mathcal{U}^k)\delta\mathcal{U}^{k+1} = b(\mathcal{U}^n, \mathcal{U}^k) \qquad (12)$$

where $\mathcal{U} = (U_1, \ldots, U_N)^t$.

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The test cases

- Detonation in a closed box
- Lid driven cavity flows

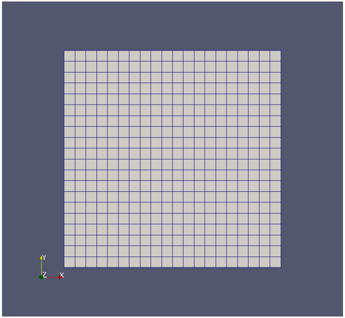
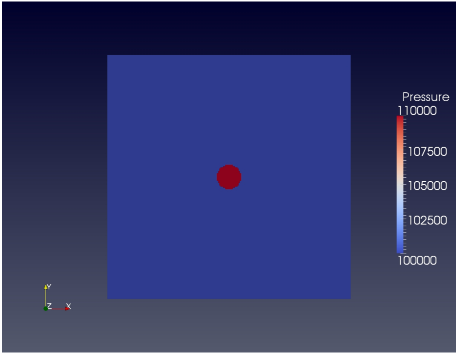


Figure: Mesh

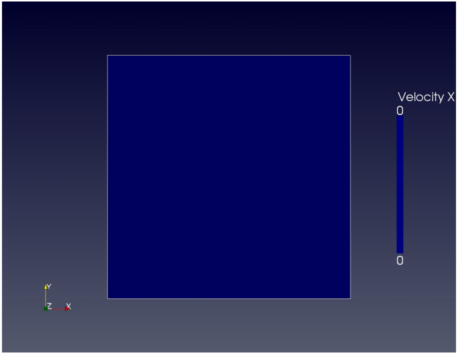
Initial data

Detonation problem
$\vec{v} = \vec{0}$
$T = 300K$
Fixed walls
200×200 grid



Initial data

Lid driven cavity
$\vec{v} = \vec{0}$
$T = 35K$
3 fixed walls
1 moving wall
50×50 grid



Explicit vs Implicit: Lid driven cavity

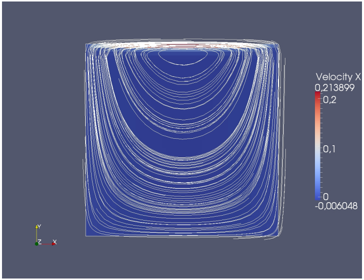


Figure: Explicit scheme, Stationnary regime

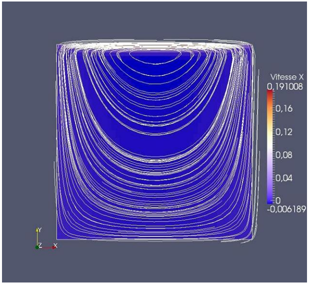


Figure: cfl 1600 nb time steps 1

CFL	0.5	100	400	800	1600
Number of time steps	3152	16	4	2	1
Time of computation	155.987	3.55	1.079	0.634	0.34

Upwind vs Centered: Lid driven cavity

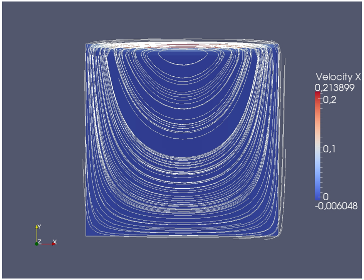


Figure: Upwind scheme, Stationnary regime

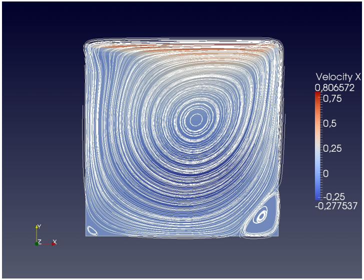


Figure: Centered scheme, Stationnary regime

The centered scheme is much less diffusive and captures the correct solution as opposed to the upwind scheme.

Scaling strategy

- For a better preconditioning of the matrix, off diagonal entries of the matrix must have a small magnitude
- After applying a similarity transformation with a diagonal matrix D_{sca} and D_{sca}^{-1}, all entries of the matrix have the same magnitude.
- Instead of solving system $\mathcal{A}\delta\mathcal{U} = b$, one can rather solve:

$$\tilde{\mathcal{A}}\delta\tilde{\mathcal{U}} = \tilde{b}, \tag{13}$$

where $\tilde{\mathcal{A}} = D_{sca}\mathcal{A}D_{sca}^{-1}$, $\delta\tilde{\mathcal{U}} = D_{sca}\delta\mathcal{U}$ and $\tilde{b} = D_{sca}b$.

- System (13) can be resolved more easily using an ILU preconditioner.

T.H.Dao, M. Ndjinga, F. Magoules, Comparison of Upwind and Centered Schemes for Low Mach Number Flows, *Finite Volumes for Complex Application VI*, Prague, June 6-10, 2011.

Scaling strategy

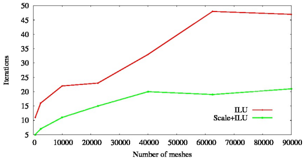


Figure: Number of GMRES iterations for the upwind scheme, CFL 1000

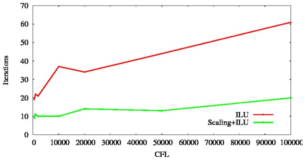


Figure: Number of GMRES iterations for the upwind scheme, mesh 100×100

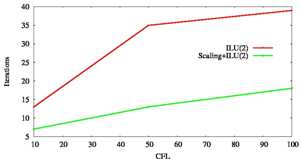


Figure: Number of GMRES iterations for the centered scheme.

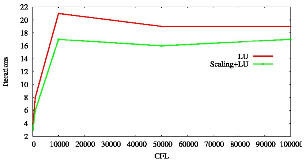


Figure: Number of Newton iterations for the centered scheme.

THANK YOU FOR YOUR ATTENTION!