Relaxation method based solvers for multifluid flows

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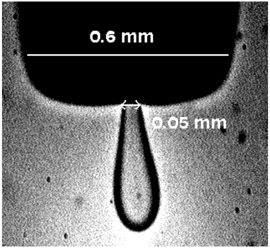
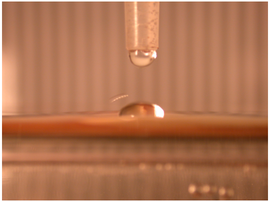
Headlines

Physical context

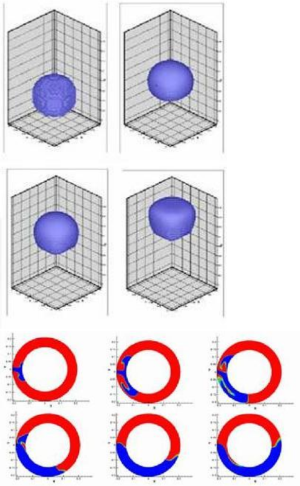
- Two fluids
  liquid or gas
  different physical properties (EOS)
  non-miscible fluids, separated by interfaces
  surface tension force
  viscous fluids
- Compressibility
  acoustic wave propagation (interface deformation)
  fluid volume variation
- Low Mach flows
  low fluid velocities
  pressure fluctuations almost negligible





Numerical context : FLUIDBOX

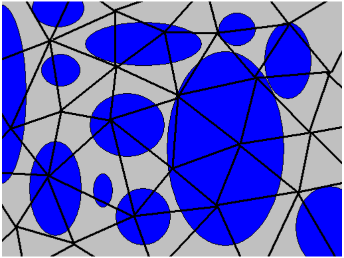
- 2D-3D
- unstructured meshes
- moving meshes
- finite volume and finite different element methods
- cell vertex, cell centered formulation
- explicit and implicit formulation
- high order MUSCL technique
- Runge Kutta schemes
- upwind downwind triangles
- parallel computing



Headlines

Fluids unknowns

- volume fraction $\alpha_k = \dfrac{V_k}{V} \in [0,1]$
- mass fraction $y_k = \dfrac{m_k}{m} \in [0,1]$
- density $\rho_k = \dfrac{m_k}{V_k}$
- velocity u_k
- internal energy ϵ_k
- energy $E_k = \rho_k \left(\epsilon_k + \dfrac{1}{2}|u_k|^2 \right) > 0$
- enthalpy $H_k = \dfrac{E_k + p_k}{\rho_k}$
- temperature T_k
- entropy S_k
- sound speed c_k



Reduced model : Kapila(2000)

- Baer Nunziato model : u_k, p_k, velocity and pressure relaxation procedure
- asymptotic expansion : $u_k = u + \epsilon u_k^{'}$, $p_k = p + \epsilon p_k^{'}$

$$\left\{ \begin{array}{l} \partial_t(\alpha_k) + u\partial_x(\alpha_k) + \beta_k\partial_x(u) = 0 \\ \\ \partial_t(\mathbf{w}) + \partial_x(\mathbf{f}) = 0 \end{array} \right.$$

$$\mathbf{w} = \begin{pmatrix} \alpha_k\rho_k \\ \rho u \\ E \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} \alpha_k\rho_k u \\ \rho u^2 + p \\ (E+p)u \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} \rho_k \\ u \\ p \end{pmatrix}$$

- mixture density $\rho = \sum_k \alpha_k\rho_k$
- compaction term $\beta_k = \alpha_k\alpha_{k'} \dfrac{\rho_k c_k^2 - \rho_{k'} c_{k'}^2}{\alpha_{k'}\rho_k c_k^2 + \alpha_{k'}\rho_k c_k^2}$
- sound speed $\dfrac{1}{\rho c^2} = \sum_k \dfrac{\alpha_k}{\rho_k c_k^2}$
- entropy $S = \sum y_k S_k$

'Stiffened gas' equation of states

- pressure : $p + \gamma P^{\infty} = (\gamma - 1)\rho(\epsilon - \epsilon^{\infty})$

$$\frac{1}{\gamma - 1} = \sum_k \frac{\alpha_k}{\gamma - 1}, \quad \frac{\gamma p^{\infty}}{\gamma - 1} = \sum_k \frac{\alpha_k \gamma_k p_k^{\infty}}{\gamma_k - 1}, \quad \epsilon^{\infty} = \sum_k y_k \left(\epsilon_{k0} - \frac{p_{k0} + \gamma_k p_k^{\infty}}{\rho_{k0}(\gamma_k - 1)} \right)$$

- temperature : $p + p_k^{\infty} = (\gamma_k - 1)\rho_k^{\gamma_k} C_{vk} \left(\frac{T_k}{\rho_k^{\gamma_k - 1}} - \frac{T_k^{\infty}}{\rho_{k0}^{\gamma_k - 1}} \right)$

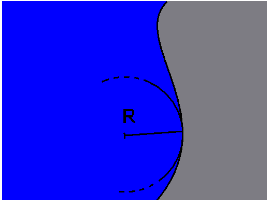
$$T_k^{\infty} = T_{k0} - \frac{p_{k0} + p_k^{\infty}}{\rho_{k0}(\gamma_k - 1) C_{vk}}$$

- sound speed : $\rho_k c_k^2 = \gamma_k (p + p_k^{\infty})$, entropy : $S_k = (p + p_k^{\infty})/(\rho_k^{\gamma_k})$

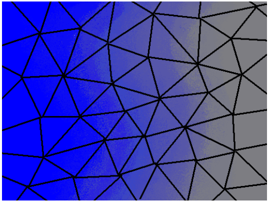
	γ	P^{∞}	ρ_0	P_0	ϵ_0	T_0	C_v
air	1.4	0	50	$1.0\ 10^5$	$2.0\ 10^5$	300	$1.0\ 10^3$
water	4.4	$6.0\ 10^8$	$1.0\ 10^3$	$1.0\ 10^5$	$6.17\ 10^5$	220	$4.18\ 10^3$

Capillary effects

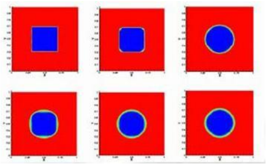
Continuum Surface Force (CSF, Brackbill 1992)



$\Longrightarrow$



- ϕ_k phase field α_k, y_k
- $n = \nabla \phi_k$ normal at the interface
- $\kappa = \nabla \cdot \left(\frac{n}{|n|} \right)$ curvature
- σ surface tension coefficient
- $F_S = -\sigma \kappa n$ surface tension force



Headlines

'hyper-consistent' schemes

Proposition

- *when α_k is constant, the system becomes conservative :*

$$\partial_t(\mathbf{w}) + \nabla \cdot (\mathbf{f}) = 0$$

$\longrightarrow$ *the discretisation of the numerical flux* $\mathbf{f}$ *must be in a conservative form.*

- *when the solution $\overline{\mathbf{w}}$ is such that $(\overline{\rho_k}, \overline{u}, \overline{p})$ are constant, the volume fraction and masses equations are redundant. This criterion leads to an 'hyper-consistent' dicretisation of the non-conservative operator.*

'hyper consistent' numerical schemes rewrite formally as :

$$\begin{cases} \dfrac{(\alpha_k)_i^{n+1} - (\alpha_k)_i^n}{\Delta t} + (\mathbf{u} \cdot \nabla)_i^h \alpha_k + (\beta_k \cdot \nabla)_i^h \mathbf{u} = 0 \\ \dfrac{\mathbf{w}_i^{n+1} - \mathbf{w}_i^n}{\Delta t} + \dfrac{\boldsymbol{\phi}_{i+1/2}^n - \boldsymbol{\phi}_{i-1/2}^n}{\Delta x} = 0 \end{cases}$$

$$\rightarrow \boldsymbol{\phi}_{i+1/2}^n = \frac{1}{2}\left[\mathbf{f}_{i+1}^n + \mathbf{f}_i^n - \mathbf{P}|\Lambda|\mathbf{P}^{-1}(\mathbf{w}_{i+1}^n - \mathbf{w}_i^n)\right]$$

$$\rightarrow (\mathbf{u} \cdot \nabla)_i^h \alpha_k = \frac{\boldsymbol{\phi}_{i+1/2}^{\alpha_k \rho_k}\left(\alpha_k^n, \overline{\mathbf{w}}^n\right) - \boldsymbol{\phi}_{i-1/2}^{\alpha_k \rho_k}\left(\alpha_k^n, \overline{\mathbf{w}}^n\right)}{\Delta x}$$

Pressure relaxation solver

$$\partial_t(\mathbf{W}_R) + \partial_x(\mathbf{F}_R) + B_R\partial_x(\mathbf{V}_R) = \frac{1}{\lambda}\mathbf{R}$$

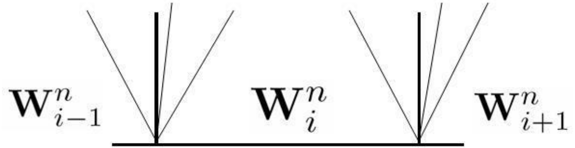
$$\mathbf{W}_R = \begin{pmatrix} \alpha_k \\ \alpha_k\rho_k \\ \rho\mathbf{u} \\ E \\ \pi \end{pmatrix}, \quad \mathbf{B}_R = \begin{pmatrix} \mathbf{u} & 0 & \tilde{\beta}_k & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a^2/\rho & 0 & \mathbf{u} \end{pmatrix}, \quad \mathbf{F}_R = \begin{pmatrix} 0 \\ \alpha_k\rho_k\mathbf{u} \\ \rho\mathbf{u}^2 + \pi \\ (E+\pi)\mathbf{u} \\ 0 \end{pmatrix}$$

$$\mathbf{V}_R = \begin{pmatrix} \alpha_k \\ \rho_k \\ \mathbf{u} \\ \epsilon \\ \pi \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ p - \pi \end{pmatrix}$$

- relaxation pressure $\pi \longrightarrow p$
- relaxation time $\lambda \longrightarrow 0$
- relaxation parameter $a > \rho c$
- approximate compaction $\tilde{\beta}^k = \alpha_k - \frac{y_k a_k^2}{a^2}$

wave	Riemann invariants					
λ_u	u			π		
$\lambda_{u\pm a/\rho}$	$u \pm a\rho$	$\pi \mp au$	$\pi^2 - 2a^2\epsilon$	y_k	$(\alpha_k - y_k a^2/a_k^2)/\rho$	a

1-D numerical implementation of relaxation schemes



exact solution :

$$\mathcal{V}_{i-1/2}(x) = \mathcal{V}\left(\frac{x - x_{i-1/2}}{\Delta t}, \mathbf{W}_{i-1}^n, \mathbf{W}_i^n\right)$$

Godunov method :

$$\Delta x \mathbf{W}_i^{n+1} = \int_{x_{i-1/2}}^{x_i} \mathcal{V}_{i-1/2}(x)dx + \int_{x_i}^{x_{i+1/2}} \mathcal{V}_{i+1/2}(x)dx$$

wave propagation form :

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n - \frac{\Delta t}{\Delta x}\left[\left(\overline{\mathbf{A}}^- \Delta \mathbf{W}\right)_{i+1/2}^n + \left(\overline{\mathbf{A}}^+ \Delta \mathbf{W}\right)_{i-1/2}^n\right]$$

$$\left(\overline{\mathbf{A}}^- \Delta \mathbf{W}\right)_{i+1/2}^n = -\frac{1}{\Delta t}\int_{x_i}^{x_{i+1/2}} \left(\mathcal{V}_{i+1/2}(x) - \mathbf{W}_i^n\right) dx$$

$$\left(\overline{\mathbf{A}}^+ \Delta \mathbf{W}\right)_{i-1/2}^n = -\frac{1}{\Delta t}\int_{x_{i-1/2}}^{x_i} \left(\mathcal{V}_{i-1/2}(x) - \mathbf{W}_i^n\right) dx$$

'hyper-consistent' schemes properties

update solution :

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n - \frac{\Delta t}{\Delta x}(\boldsymbol{\psi}_{i+1/2} - \boldsymbol{\psi}_{i-1/2})$$

'hyper consistency' formulation :

$$\boldsymbol{\psi}_{i+1/2} = \boldsymbol{\phi}_{i+1/2} + \left(\overline{\mathbf{B}}^{-}\Delta\mathbf{V}\right)_{i+1/2}^{n}, \quad \boldsymbol{\psi}_{i-1/2} = \boldsymbol{\phi}_{i-1/2} - \left(\overline{\mathbf{B}}^{+}\Delta\mathbf{V}\right)_{i-1/2}^{n}$$

dissipative formulation :

$$\boldsymbol{\psi}_{i+1/2} = \frac{1}{2}\left[\mathbf{F}_i^n + \mathbf{F}_{i+1}^n - \left(|\overline{\mathbf{A}}|\Delta\mathbf{W}\right)_{i+1/2}^n - \left(|\overline{\mathbf{B}}|\Delta\mathbf{V}\right)_{i+1/2}^n\right] + \frac{1}{2}\left(\overline{\mathbf{B}}\Delta\mathbf{V}\right)_{i+1/2}^n$$

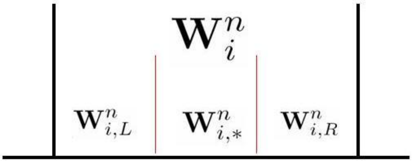
$$\boldsymbol{\psi}_{i-1/2} = \frac{1}{2}\left[\mathbf{F}_{i-1}^n + \mathbf{F}_i^n - \left(|\overline{\mathbf{A}}|\Delta\mathbf{W}\right)_{i-1/2}^n - \left(|\overline{\mathbf{B}}|\Delta\mathbf{V}\right)_{i-1/2}^n\right] - \frac{1}{2}\left(\overline{\mathbf{B}}\Delta\mathbf{V}\right)_{i-1/2}^n$$

Proposition

There exists a matrix $\overline{\mathbf{B}}$ such that approximate solvers associated to 'hyper consistent' numerical schemes satisfy :

$$\sum_k (\delta\mathcal{V})_k = \Delta\mathbf{F} + \overline{\mathbf{B}}\Delta\mathbf{V}$$

2^{nd} order space accuracy



gradients construction :

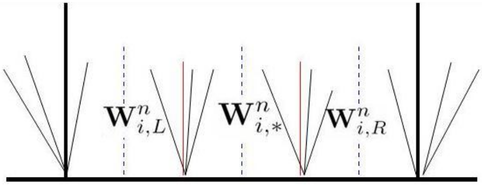
$$\nabla \mathbf{W}_{i,R}^n = Lim\left(\frac{\mathbf{W}_{i+1} - \mathbf{W}_{i-1}}{2\Delta x}, \frac{(\Delta \mathbf{W})_{i+1/2}}{x}\right), \quad \nabla \mathbf{W}_{i,L}^n = Lim\left(\frac{\mathbf{W}_{i+1} - \mathbf{W}_{i-1}}{2\Delta x}, \frac{(\Delta \mathbf{W})_{i-1/2}}{\Delta x}\right)$$

states reconstruction :

$$\mathbf{W}_{i,R}^n = \mathbf{W}_i^n + \frac{\Delta x}{2}\nabla \mathbf{W}_{i,R}^n, \quad \mathbf{W}_{i,L}^n = \mathbf{W}_i^n - \frac{\Delta x}{2}\nabla \mathbf{W}_{i,L}^n$$

conservation property : $\mathbf{W}_i^n = \frac{1}{3}(\mathbf{W}_{i,L}^n + \mathbf{W}_{i,*}^n + \mathbf{W}_{i,R}^n)$

2^{nd} order implementation



$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n - \frac{\Delta t}{\Delta x}\left[H_{i+1/2} - H_{i_1/2}\right]$$

second order flux formulation :

$$H^n_{i-1/2} = \mathbf{F}^n_{i,L} + \mathbf{B}^n_i \mathbf{W}^n_{i,L} + \frac{1}{\Delta t}\int_{x_{i-1/3}}^{x_{i-1/2}} \left[\mathcal{V}\left(\frac{x - x_{i-1/2}}{\Delta t}, \mathbf{W}^n_{i-1,R}, \mathbf{W}^n_{i,L}\right) - \mathbf{W}^n_{i,L}\right] dx$$

$$H^n_{i+1/2} = \mathbf{F}^n_{i,R} + \mathbf{B}^n_i \mathbf{W}^n_{i,R} - \frac{1}{\Delta t}\int_{x_{i+1/3}}^{x_{i+1/2}} \left[\mathcal{V}\left(\frac{x - x_{i+1/2}}{\Delta t}, \mathbf{W}^n_{i,R}, \mathbf{W}^n_{i+1,L}\right) - \mathbf{W}^n_{i,R}\right] dx$$

Second order

- second order time accuracy : default correction :

prediction : $\mathbf{W}_i^{n+1/2} = \mathbf{W}_i^n - \frac{\Delta t}{a_i} \sum_{j \in \nu(i)} \phi_{ij,ji}^n$

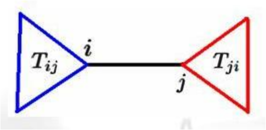
correction : $\mathbf{W}_i^{n+1} = \frac{1}{2} \left(\mathbf{W}_i^{n+1/2} + \mathbf{W}_i^n - \frac{\Delta t}{a_i} \sum_{j \in \nu(i)} \phi_{ij,ji}^{n+1/2} \right)$

- 2D second order space accuracy :
  MUSCL technique :

$$\nabla \mathbf{W}_{ij} = \frac{1}{2} \left(\nabla \mathbf{W}_{ij}^{cent} + \nabla \mathbf{W}_{ij}^{up} \right) \cdot \boldsymbol{\eta}_{ij}$$

Van Albada Van Leer limiter :

$$\mathbf{W}_{ij} = \mathbf{W}_i + \frac{1}{2} Lim(\nabla \mathbf{W}_{ij}, \nabla \mathbf{W}_{ij}^{cent} \cdot \boldsymbol{\eta}_{ij})$$



Source terms

- splitting technique

$$\begin{cases} \partial_t(\alpha_k) = 0 \\ \partial_t(\alpha_k \rho_k) = 0 \\ \partial_t(\rho \mathbf{u}) = \rho \mathbf{g} + F_S + \nabla \cdot \tau \\ \partial_t(E) = (\rho \mathbf{g} + F_S) \cdot \mathbf{u} + \nabla \cdot (\tau \mathbf{u}) \end{cases}$$

- $\mathbf{g}$ gravity
- F_S surface force
- $\tau = \frac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$ viscosity stress tensor
- $\frac{1}{\mu} = \sum_k \frac{\alpha_k}{\mu_k}$ mixture viscosity coefficient

Low Mach preconditioning

- Low Mach number : $Ma = \frac{|\mathbf{u}|}{c} << 1$
- solutions spoiled by rounded errors coming from acoustic wave resolution
- Turkel pressure preconditioning method (rounded errors filter) :

$$\frac{1}{Ma^2}\partial_t(p) + \mathbf{u}\cdot\nabla(p) + \rho c^2\nabla\cdot(\mathbf{u}) = 0$$

- preconditioned relaxation system :

$$\begin{cases} \partial_t(\alpha_k) + \mathbf{u}\cdot\nabla(\alpha_k) + \tilde{\beta}_k\nabla\cdot(\mathbf{u}) = 0 \\ \partial_t(\alpha_k\rho_k) + \nabla\cdot(\alpha_k\rho_k\mathbf{u}) = 0 \\ \partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}^2 + \pi) = 0 \\ \partial_t(E) + \nabla\cdot((E+\pi)\mathbf{u}) = 0 \\ \partial_t(\pi) + \left(\mathbf{u} + \frac{a^R - a^L}{\rho}\right)\cdot\nabla(\pi) + \frac{a^R a^L}{\rho}\nabla\cdot(\mathbf{u}) = \frac{1}{\lambda}(p-\pi) \end{cases}$$

- L.D., waves : $\lambda^{\pm} \approx \frac{(M^2+1)u \pm \sqrt{(M^2-1)^2u^2 + 4M^2c^2}}{2}$

Implicit formulation

- implicit formulation

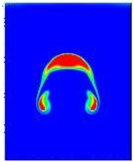
$$\left(1 + \frac{\Delta t}{a_i} \sum_{j \in \nu(i)} \mathbf{A}^+_{ij} \cdot \boldsymbol{\eta}_{ij}\right) (\mathbf{W}_i^{n+1} - \mathbf{W}_i^n) + \sum_{j \in \nu(i)} \mathbf{A}^+_{ji} \cdot \boldsymbol{\eta}_{ji} (\mathbf{W}_j^{n+1} - \mathbf{W}_j^n) = -\frac{\Delta t}{a_i} \psi_{ij}^n$$

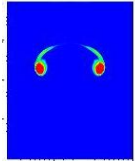
- Acoustic scheme (Guillard, Murrone)

$$\mathbf{A}^+_{ij} = \left(\frac{\partial \mathbf{F}^*_{ij}}{\partial \mathbf{W}^*_{ij}} + \mathbf{B}(\mathbf{W}_i^n)\right) \left(\frac{\partial \mathbf{W}^*_{ij}}{\partial \mathbf{W}^*_i}\right)$$

- Resolution based on iterative methods :

  Jacobi
  Gauss-Seidel
  Gmres

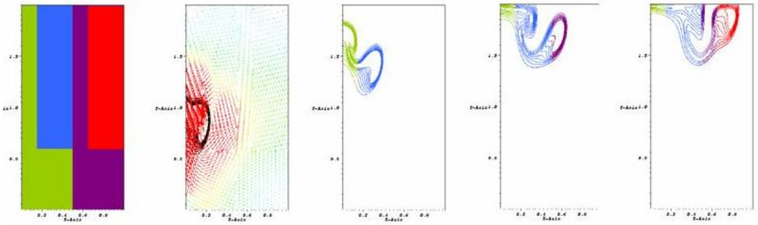




Headlines

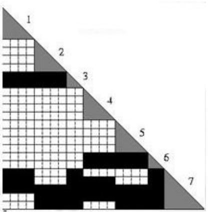
Fluidbox parallelisation

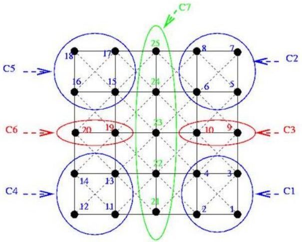
- parallelisation based on mesh partitioning
- block Gauss Seidel or block Jacobi preconditioners
- dedicated parallel assembly implementation
- partitioning step is performed by Metis
- overlap the frontiers of domain decomposition

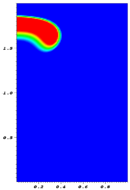


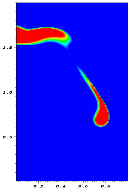
PASTIX : direct solver and graph partitioner

- PASTIX : parallel direct solver based on LU method
  robust factorisation (ill conditioned matrix)
  unsymmetric matrix with symmetric pattern
- PASTIX features
  matrix ordering techniques based on graph partitioning :
    incomplete Nested Dissection
    approximate Minimum Degree method
  benefits :
    minimising the fill-in in the factorized matrix and the number of operations
    maximising the independence of computations
  block symbolic factorisation :
    compute the block pattern of the factorized matrix(liner time complexities)
    block data structure allow to use dense linear algebra subroutine (BLAS3)



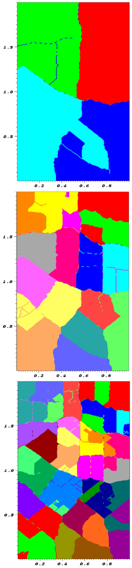






PASTIX efficiency

Mesh Unknows	101 × 201 121806	201 × 401 483606	401 × 801 1927206
4 processors			
PASTIX	$1.41\ 10^3$	$1.59\ 10^4$	— — ——
Gauss-Seidel 10^{-3}	$4.77\ 10^4$	$4.05\ 10^5$	$3.38\ 10^6$
Gauss-Seidel 10^{-5}	$7.13\ 10^4$	$5.57\ 10^5$	— — ——
Gmres 10^{-3}	$5.95\ 10^3$	$4.78\ 10^4$	$4.18\ 10^5$
Gmres 10^{-5}	$5.22\ 10^4$	$4.23\ 10^5$	— — ——
16 processors			
PASTIX	$6.10\ 10^2$	$5.65\ 10^3$	$6.17\ 10^4$
Gauss-Seidel 10^{-3}	$1.63\ 10^4$	$1.55\ 10^5$	$1.32\ 10^6$
Gauss-Seidel 10^{-5}	$2.46\ 10^4$	$2.12\ 10^5$	$1.53\ 10^7$
Gmres 10^{-3}	$2.07\ 10^3$	$1.82\ 10^4$	$1.32\ 10^5$
Gmres 10^{-5}	$1.80\ 10^4$	$1.65\ 10^5$	$1.84\ 10^6$
32 processors			
PASTIX	$6.30\ 10^2$	$5.71\ 10^3$	$6.31\ 10^4$
Gauss-Seidel 10^{-3}	$8.15\ 10^3$	$9.14\ 10^4$	$1.46\ 10^5$
Gauss-Seidel 10^{-5}	$1.23\ 10^4$	$1.26\ 10^5$	$9.74\ 10^5$
Gmres 10^{-3}	$1.04\ 10^3$	$1.07\ 10^4$	$7.76\ 10^4$
Gmres 10^{-5}	$8.83\ 10^3$	$9.67\ 10^4$	$1.12\ 10^5$



Headlines

Conclusion

- Done
  'hyper consistent' numerical schemes (relaxation scheme)
  second order extension
  low Mach preconditioning
  implicit formulation
  parallel computing : Pastix
- In progress
  3D
  comparison with experiments