Two phase flow simulations based on Immersed boundary method by utilizing MUMPS solver

Yuri Feldman, MUMPS User Days, Grenoble, France, June 2017



Outline

- 1. History of using MUMPS
- 2. Motivation of the Research
- 3. Governing Equations
- 4. Numerical Method
- 5. Direct Numerical Simulations
 - o Rising bubble
 - o Droplet Relaxation to Disk
- 6. Future Optimization Strategies
- 7. Conclusions and Wish List



Fully Pressure – Velocity Coupling

 $\nabla \cdot \boldsymbol{u} = 0$ $\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \frac{1}{Gr^{0.5}}\nabla^2 \boldsymbol{u} + \theta \overrightarrow{e_z}$ $\frac{\partial \theta}{\partial t} + (\boldsymbol{u} \cdot \nabla)\theta = \frac{1}{PrGr^{0.5}}\nabla^2 \theta$

- No extra prediction-correction step for pressure is required
- ✓ Large Indefinite ill conditioned matrix

(Feldman, Gelfgat, Computers&Structures, 2009)



Sequential version of MUMPS

✓ Very efficient for 2D problems

Immersed Boundary (IB) Method

- Simulation of flows in the presence of complex geometries and moving boundaries.
- Straight forward computation of the forces/heat fluxes acting on the immersed boundary.
- The implementation of the method requires very limited modifications of the existing time stepping/linear stability codes.



Concept of IB Method



Regularization operator to smear force.

Interpolation operator to interpolate velocity



Implicit IB Method Based on Fully Pressure – Velocity Coupling

Time marching solver.

Steady state solver.

Generalized eigenvalue solver.



Fully Coupled IB Time Marching Solver

$$\begin{bmatrix} H_u & 0 & -\nabla_p^x & R(\vec{F_x}) & 0 \\ 0 & H_v & -\nabla_p^y & 0 & R(\vec{F_y}) \\ \nabla_u^x & \nabla_v^y & 0 & 0 & 0 \\ I(u) & 0 & 0 & 0 & 0 \\ 0 & I(v) & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u^{(n+1)} \\ v^{(n+1)} \\ p^{(n+1)} \\ F_x^{(n+1)} \\ F_y^{(n+1)} \end{bmatrix} = \begin{bmatrix} R_u^{(n)} \\ R_v^{(n)} \\ R_p^{(n)} \\ U_b \\ V_b \end{bmatrix}$$

Immersed boundary formulation

+ Dirichlet point for pressure

 $\overrightarrow{F_x}$ and $\overrightarrow{F_y}$ play a role of Lagrange multipliers

- Extremely efficient for 2-D, axi-symmetric problems.
- Open source MUltifrontal Massively Parallel sparse direct Solver (MUMPS, httt://mumps.enseeiht.fr/) is used for LU decomposition.

Qualitative verification

Wake characteristics, Re=200

Feldman&Gulberg, JCP, 2016

Carmo et al. JFM (2009)



Fully Coupled IB Steady State Solver

Newton iterations:

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 MUltifrontal Massively Parallel sparse direct Solver (MUMPS, htt://mumps.enseeiht.fr/) is used for LU decomposition.

Flow around cylinder -verification

Definition of the characteristic dimensions for the wake structure



Comparison of the wake characteristics

<i>Re=20</i>		l/d	a/d	b/d	θ	C_D
	Feldman&Gulberg, JCP, 2016	0.95	0.37	0.43	42.9 ⁰	2.09
	Taira and Colonius (2007)	0.94	0.37	0.43	43.3 ⁰	2.06
	Linnick and Fasel (2005)	0.93	0.36	0.43	43.5 ⁰	2.06
	Dennis and Chung (1970)	0.94	-	-	43.7	2.05
Re=40						
	Feldman&Gulberg, JCP, 2016	2.31	0.72	0.60	52.3 ⁰	1.56
	Taira and Colonius (2007)	2.30	0.73	0.60	53.7 ⁰	1.54
	Linnick and Fasel (2005)	2.28	0.72	0.60	53.6 ⁰	1.54
	Dennis and Chung (1970)	2.35	-	-	53.8	1.52

Re=20

Re=40



Eigenvalue Problem

Generalized eigenvalue problem with IB formalism where J is the Jacobian matrix and detB=0



$$(\boldsymbol{J}-\sigma\boldsymbol{B})^{-1}\boldsymbol{B}\big(\tilde{\boldsymbol{u}},\tilde{\boldsymbol{v}},\tilde{\boldsymbol{p}},\tilde{\boldsymbol{\theta}},\tilde{\boldsymbol{F}}_{\boldsymbol{x}},\tilde{\boldsymbol{F}}_{\boldsymbol{y}},\tilde{\boldsymbol{Q}}\big)=\mu\big(\tilde{\boldsymbol{u}},\tilde{\boldsymbol{v}},\tilde{\boldsymbol{p}},\tilde{\boldsymbol{\theta}},\tilde{\boldsymbol{F}}_{\boldsymbol{x}},\tilde{\boldsymbol{F}}_{\boldsymbol{y}},\tilde{\boldsymbol{Q}}\big),\ \mu=\frac{1}{\lambda-\sigma}$$

Inverse of shifted Jacobian matrix

Arpack library,

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http://www.caam.rice.edu/software/ARPACK is used for performing Arnoldi iteration.

Flow around the Cylinder-Linear Stability Analysis

The most unstable mode of vorticity, Re=100



Two Phase Flows

- Biomechanical engineering
 - Modeling cells motility in human body
 - Modeling tumor growth
- Optical wave guides
 - Tapered fiber bundle



[1] Cells division



[2] Seven fiber structure which allows to achieve good quality beam

[1] http://www.wisegeekhealth.com/what-is-the-connection-between-the-cell-cycle-and-cancer.htm [2] http://soreq.gov.il/mmg/Pages/



Purpose of the Present Research

• Major Objective:

To develop a **robust and efficient** numeric tool which represents the **underlying physical processes** inherent to two phase flow.

- Challenges:
 - To consistently provide preservation of initial volume of both phases.
 - To implicitly couple between the interface curvature and the velocity field.



Governing Equations

Mass conservation

$$\nabla \cdot \widetilde{\boldsymbol{u}} = 0$$

Navier Stokes

$$\rho_r(I)\left(\frac{\partial \widetilde{\boldsymbol{u}}}{\partial \widetilde{t}} + \widetilde{\boldsymbol{u}} \cdot \boldsymbol{\nabla} \widetilde{\boldsymbol{u}}\right) =$$

$$= -\nabla \tilde{p} + \frac{\rho_r}{Re\mu_r} \nabla \cdot \left(\mu_r(I) (\nabla \tilde{u} + (\nabla \tilde{u})^T) \right) + \frac{\rho_r}{We} \int_{\Gamma} \frac{\partial^2 \tilde{X}_f}{\partial \tilde{S}^2} - \rho_r(I)$$

$$_{Re} = \frac{\rho_H U_g D}{\mu_H} \qquad We = \frac{\rho_H U_g^2 D}{\sigma}$$



Fully Coupled IB Time Marching Solver

$$\frac{\rho_r \mu_r(I)}{Re\mu_r} \nabla^2 \widetilde{\boldsymbol{u}}^{n+1} - \frac{3\rho_r(I)\widetilde{\boldsymbol{u}}^{n+1}}{2\Delta \widetilde{t}} - \nabla p + \frac{\rho_r}{We} \int_{\Gamma} \frac{\partial^2 \widetilde{\boldsymbol{X}}_f}{\partial \widetilde{S}^2} = \rho_r(I) \left(\frac{-4\widetilde{\boldsymbol{u}}^n + \widetilde{\boldsymbol{u}}^{n-1}}{2\Delta \widetilde{t}} + \widetilde{\boldsymbol{u}}^n \cdot \nabla \widetilde{\boldsymbol{u}}^n \right) + \begin{bmatrix} 0\\1 \end{bmatrix} \rho_r(I)$$

• The fully pressure velocity coupled direct (FPCD) solver (*Feldman & Gelfgat 2009*).

$$\begin{bmatrix} H_u & 0 & -\nabla_p^x & \frac{\rho_r}{We} R\left(\frac{\partial^2 \tilde{X}_f}{\partial \tilde{S}^2}\right) & 0 \\ 0 & H_v & -\nabla_p^y & 0 & \frac{\rho_r}{We} R\left(\frac{\partial^2 \tilde{Y}_f}{\partial \tilde{S}^2}\right) \\ \nabla_u^x & \nabla_v^y & 0 & 0 & 0 \\ Int(\tilde{u}) & 0 & 0 & -1 & 0 \\ 0 & Int(\tilde{v}) & 0 & 0 & 0 \\ \end{bmatrix} \begin{bmatrix} \tilde{u}^{(n+1)} \\ \tilde{v}^{(n+1)} \\ \tilde{\rho}^{(n+1)} \\ \tilde{\rho}^{(n$$

Immersed boundary formulation



Curvature as Lagrange Multiplier

$$\begin{bmatrix} H_{u} & 0 & -\nabla_{p}^{x} & \frac{\rho_{r}}{We} R\left(\frac{\partial^{2} \tilde{X}_{f}}{\partial \tilde{S}^{2}}\right) & 0 \\ 0 & H_{v} & -\nabla_{p}^{y} & 0 & \frac{\rho_{r}}{We} R\left(\frac{\partial^{2} \tilde{Y}_{f}}{\partial \tilde{S}^{2}}\right) \\ \nabla_{u}^{x} & \nabla_{v}^{y} & 0 & 0 & 0 \\ Int(\tilde{u}) & 0 & 0 & -1 & 0 \\ 0 & Int(\tilde{v}) & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \tilde{u}^{(n+1)} \\ \tilde{v}^{(n+1)} \\ \frac{\partial}{\tilde{S}^{2}} \\ \frac{\partial}{\partial \tilde{S}^{2}} \\ \frac{\partial}{\partial \tilde{S}^{2}} \\ \frac{\partial}{\partial \tilde{S}^{2}} \end{bmatrix} = \begin{bmatrix} R_{u}^{(n)} \\ R_{v} \\ R_{p} \\ R_{fy} \end{bmatrix}$$
 Immersed boundary formulation

$$\begin{pmatrix} 0 & Af \\ \overline{\partial S^2} \end{pmatrix} = \frac{(A_{l+1} - 2A_l + A_{l-1})}{(\Delta S)^2}$$

$$\frac{\Delta T (Int(u)_{l+1}^{n+1} - 2Int(u)_l^{n+1} + Int(u)_{l-1}^{n+1})}{2(\Delta S)^2} - \left(\frac{\partial^2 X}{\partial S^2}\right) =$$

$$\frac{-X_{l+1}^n + 2X_l^n - X_{l-1}^n}{(\Delta S)^2} + \frac{\Delta T (-Int(u)_{l+1}^n + 2Int(u)_l^n - Int(u)_{l-1}^n)}{2(\Delta S)^2}$$
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Runge Kutta 2 $X_l^{n+1} = X_l^n + (K_1 + K_2)/2$ $K_1 = \Delta T \cdot Int(u)_{l(X_l,Y_l)}^n$ $K_2 = \Delta T \cdot Int(u)_{l(X_l^n + K_1,Y_l^n + K_1)}^{n+1}$

Indicator Function

• Far from the interface:

$$I(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \text{ is in fluid } A \\ 0, & \text{if } \mathbf{x} \text{ is in fluid } B \end{cases}$$

• Near the interface

$$(\nabla I)_{i,j} = \sum_{l} n_{l} \delta^{2}(r_{x}, r_{y}) \Delta s_{l},$$

 $\nabla^{2} I = \nabla \cdot \sum_{l} n_{l} \delta^{2}(r_{x}, r_{y}) \Delta s_{l}$ Solved with MUMPS

$$(\rho_r(\mathbf{I}), \mu_r(\mathbf{I})) = (\rho_r, \mu_r - 1) \cdot \mathbf{I} + 1$$

Indicator Function, Normal $(\nabla I)_{i,i} = \sum_l \boldsymbol{n}_l \delta^2(r_x, r_y) \Delta s_l$ $\begin{bmatrix} x \\ y \end{bmatrix}(t) = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} t^2 + \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} t + \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$ $X_{(t=0)} = X_{l-1}$, $X_{(t=\Delta s_l)} = X_l$, $X_{(t=\Delta s_{l+1}+\Delta s_l)} = X_{l+1}$ $\begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ \Delta s_l^2 & \Delta s_l & 1 \\ (\Delta s_l + \Delta s_{l+1})^2 & \Delta s_l + \Delta s_{l+1} & 1 \end{bmatrix} \begin{bmatrix} X_{l-1} \\ X_l \\ X_{l+1} \end{bmatrix}$ $\boldsymbol{n}_{l} = \left(\frac{\frac{dy(\Delta s_{l})}{dt}}{\left[\left(\frac{dx(\Delta s_{l})}{dt}\right)^{2} + \left(\frac{dy(\Delta s_{l})}{dt}\right)^{2}}, \frac{-\frac{dx(\Delta s_{l})}{dt}}{\left[\left(\frac{dx(\Delta s_{l})}{dt}\right)^{2} + \left(\frac{dy(\Delta s_{l})}{dt}\right)^{2}}\right)$



Rising Bubble



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Rising Bubble Mesh Convergence



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Droplet Relaxation to Disk



	Max area discrepancy	$ ho_r = 1$, $\mu_r =$	L	
	8	3	5	8
3	1.61e-3	2.36e-3	2.22e-3	1.61e-3
-3	1.75e-3	1.61e-3	1.70e-3	1.75e-3
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Toward Fully 3D Flows

- Implicit coupling between Lagrangian forces and heat fluxes and the velocity and temperature fields.
- Diminishing of flow leakages through the boundaries of immersed bodies.
- Modularity and compatibility with any generic solver of the N-S equations based on the segregated pressure-velocity coupling (e.g. SIMPLE algorithm, fractional step, projection method).



Implicit Direct Forcing: General Concepts

Discrete 2nd order accuracy N-S equations with imbedded IB functionality (the SIMPLE method)

$$\begin{split} \frac{3\theta^{n+1}}{2\Delta t} &- \frac{1}{\sqrt{PrRa}} \boldsymbol{L}(\theta^{n+1}) - \boldsymbol{R}(Q^k(\boldsymbol{X}^k)) = \frac{4\theta^n - \theta^{n-1}}{2\Delta t} - \boldsymbol{N}(\theta^n, \boldsymbol{u}^n) + \theta^n \vec{e}_s \\ \frac{3\boldsymbol{u}^*}{2\Delta t} &- \sqrt{\frac{Pr}{Ra}} \boldsymbol{L}(\boldsymbol{u}^*) - \boldsymbol{R}(\boldsymbol{F}^k(\boldsymbol{X}^k)) = \frac{4\boldsymbol{u}^n - \boldsymbol{u}^{n-1}}{2\Delta t} - \boldsymbol{N}(\boldsymbol{u}^n, \boldsymbol{u}^n) - \nabla p^n \\ & \Delta(\delta p) = \frac{3}{2\Delta t} \nabla \cdot \boldsymbol{u}^* \\ \boldsymbol{u}^{n+1} &= \boldsymbol{u}^* - \frac{2\Delta t}{3} \nabla(\delta p), \qquad p^{n+1} = p^n + \delta p, \end{split}$$



Implicit Direct Forcing: General Concepts, Cont.



$$[H_{\theta,u}][\theta^{n+1}, u^*] = RHS \stackrel{n-1,n}{\theta,u} \longrightarrow [H_{\theta,u}] \quad [any \ vector]$$

Efficient solver, originally developed for direct inversion of Helmholtz operator is utilized, Vitoshkin H., Gelfgat A. Yu., Commun. Comput. Phys., 2013

Schur Complement Approach

$$\begin{bmatrix} \boldsymbol{H} & \boldsymbol{R} \\ \boldsymbol{I} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\theta}, \boldsymbol{u} \\ \boldsymbol{Q}, \boldsymbol{F} \end{bmatrix} = \begin{bmatrix} RHS_{\boldsymbol{\theta}, \boldsymbol{u}}^{n-1, n} \\ \boldsymbol{\theta}_{b}, \boldsymbol{U}_{b} \end{bmatrix} \begin{bmatrix} \boldsymbol{Q}, \boldsymbol{F} \end{bmatrix} = (\boldsymbol{I}H^{-1}\boldsymbol{R})^{-1} (\boldsymbol{I}H^{-1}RHS_{\boldsymbol{\theta}, \boldsymbol{u}}^{n-1, n} - \boldsymbol{\theta}_{b}, \boldsymbol{U}_{b}) \\ [\boldsymbol{\theta}, \boldsymbol{u}] = \boldsymbol{H}^{-1} (RHS_{\boldsymbol{\theta}, \boldsymbol{u}}^{n-1, n} - \boldsymbol{R}[\boldsymbol{Q}, \boldsymbol{F}])$$

 $H^{-1}RHS^{n-1,n}_{Au}$ - Original existing solver

 $H^{-1}R$ - Action of original solver on each column of *R* (can be precomputed)

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- $IH^{-1}R$, $IH^{-1}RHS_{\theta,u}^{n-1,n}$ Sparse matrix-matrix and matrix-vector multiplications (performed by existing MKL routines)
- $^{-1}$ Small, *m*×*m* indefinite matrix, is factorized at the beginning by a direct $(\mathbf{I}\mathbf{H}^{-1}\mathbf{R})$ method (MUMPS) or solved by GMRES or AMG iterative methods

 $\boldsymbol{H}^{-1}\big(RHS_{\theta,\boldsymbol{u}}^{n-1,n}-\boldsymbol{R}[Q,\boldsymbol{F}]\big)$ - Computed by original existing solver

Verification Study 1 – Sphere in Cube



200³ structured grid

The Flow Visualization • Steady flow around the hot sphere, $Ra = 10^6$, $\delta = 0.25$ Vortical structures based Particle traces on λ_2 criterion Iso-surface of $\lambda_2 = -0.1$ **Ben-Gurion University** 28 of the Negev

Nu number Comparison

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Steady flow results

δ	Ra=10 ⁵			Ra=10 ⁶			
	Ref[1]	Ref[2]	Present	Ref[1]	Ref[2]	Present	
-0.25	13.665	13.774	13.489	20.890	21.993	20.611	
-0.2	12.931	13.058	12.768	20.631	21.862	20.517	
-0.1	12.729	13.105	12.819	20.772	22.164	21.216	
0	12.658	13.415	13.160	20.701	23.344	21.589	
0.1	12.351	13.446	13.230	20.367	22.525	21.674	
0.2	12.254	13.635	13.462	19.664	22.208	21.487	
0.25	12.944	14.426	14.277	19.721	22.393	21.757	

[1] H.Yoon, D. Yu. M. Ha, Y. Park, Three-dimensional natural convection in an enclosure with a sphere at different locations. Int. J. Heat Mass Transfer 53(2010) 3143-3155.

[2] Y. Gulberg, Y. Feldman, On laminar natural convection inside multi-layered spherical shells. Int. J. Heat Mass Transfer 91(2015) 908-921.

Conclusions and Wish List

- Over the years of research activity MUMPS has been found as a very convenient tool for analysis of a broad spectrum of CFD problems.
- MUMPS usage allows for a high flexibility in choosing and manipulating well established numerical techniques to address applications requiring transient, steady and linear stability analysis.
- It will be helpful if the MUMPS developers provide users with an automatic script for installation of the whole package with all pre-requirements, or with the prebuilt libraries for the standard Linux platforms.
- It will be very convenient to have a capability to save the factorized LU matrix on hard disk for its further utilizing.