UNSTRUCTURED MOVING PARTICLE PRESSURE MESH (UMPPM) METHOD for INCOMPRESSIBLE FLOW COMPUTATION

Presented by:

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Outline

- Governing equations
- Numerical Methods: MPS & MPPM method
- Some limitations of MPPM
- The current UMPPM method
- Test cases
- Conclusion

Governing Equations

- Continuity Equation

$$\nabla \bullet \vec{u} = 0$$

- Momentum Equation

$$\rho \frac{D\vec{u}}{Dt} = -\nabla P + \mu \nabla^2 (\vec{u}) + \vec{S}$$

- Energy Equation

$$\rho C_p \frac{DT}{Dt} = k \nabla^2 (T)$$

Basic scheme for Moving Particle Semi-implicit (MPS)

- Integrating momentum equation at particle *i*

$$\vec{u}_i^{\,n+1} = \vec{u}_i^{\,n} + \frac{1}{\rho_i}\int\left(\mu\nabla^2(\vec{u})_i + \vec{S}_i - \nabla P_i\right)dt$$

- 1st-order Explicit for viscous & Implicit for pressure:

$$\vec{u}_i^{\,n+1} = \vec{u}_i^{\,n} + \frac{\Delta t}{\rho_i}\left(\mu_i\nabla^2(\vec{u})_i^n + \vec{S}_i^{\,n} - \boxed{\nabla P_i^{n+1}}\right)$$

- Particle position update

$$\vec{r}_i^{\,n+1} = \vec{r}_i^{\,n} + \Delta t\vec{u}_i^{\,n+1}$$

Ref: Koshizuka, S. and Oka, Y. (1996), "Moving-Particle Semi-implicit method for fragmentation of incompressible fluid", Nuclear Science and Engineering, Vol. 123, pp. 421-434.

MPS: Pressure-velocity coupling

- Fractional step:
  - Explicit Viscous $$\vec{u}_i^{*} = \vec{u}_i^{n} + \frac{\Delta t}{\rho_i}\left(\mu_i \nabla^2 (\vec{u})_i^n + \vec{S}_i^{\,n}\right)$$
  - Advection (Lagrangian) $$\vec{r}_i^{\,*} = \vec{r}_i^{\,n} + \Delta t \vec{u}_i^{\,*}$$
  - Implicit pressure

$$\nabla \bullet \vec{u}_i^{n+1} = 0$$

$$\vec{u}_i^{n+1} = \vec{u}_i^{*} - \frac{\Delta t}{\rho_i}\nabla P_i^{n+1}$$

$$\frac{\Delta t}{\rho_i}\nabla^2 P_i^{n+1} = \nabla \bullet \vec{u}_i^{*} \quad \text{(PPE)}$$

$$P_i^{n+1}$$

  - Correct the position:

$$\vec{r}_i^{\,n+1} = \vec{r}_i^{\,n} + \Delta t \vec{u}_i^{\,n+1}$$

Ref: Koshizuka, S. and Oka, Y. (1996), "Moving-Particle Semi-implicit method for fragmentation of incompressible fluid", Nuclear Science and Engineering, Vol. 123, pp. 421-434.

Poisson Equation in MPS

- **“Divergence-free”** condition in the MPS work reported by **Tanaka and Masunaga (2010), JCP**

$$\frac{\Delta t}{\rho_i}\nabla^2 P_i^{n+1} = \nabla \bullet \vec{u}_i^*$$

  - Pros: smooth pressure field.
  - Cons: particle may overlap each other (volume is not conserved!)

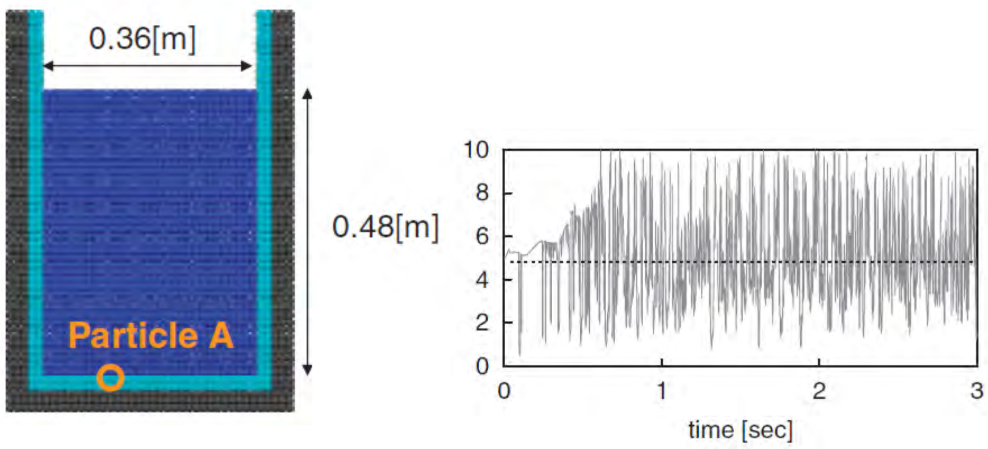
Tanaka, M. and Masunaga, T. (2010), “Stabilization and smoothing of pressure in MPS method by quasi-compressibility”, Journal of Computational Physics, Vol. 229, pp. 4279-4290.

Poisson Equation in MPS

- **"Particle Number Density"** condition: conventional MPS method

$$\frac{\Delta t}{\rho_i}\nabla^2 P_i^{n+1} = \frac{1}{\Delta t}\frac{n_i^o - n_i^*}{n_i^o}$$

- Pros: Volume can be conserved.
- Cons: Noisy pressure field.



Tanaka, M. and Masunaga, T. (2010), "Stabilization and smoothing of pressure in MPS method by quasi-compressibility", Journal of Computational Physics, Vol. 229, pp. 4279-4290.

Poisson Equation in MPS

- **Combining** both:

$$\frac{\Delta t}{\rho_i} \nabla^2 P_i^{n+1} = \nabla \bullet \vec{u}_i^* + \gamma \frac{1}{\Delta t} \frac{n_i^o - n_i^k}{n_i^o}$$

  - Pros: Volume can be conserved and smooth pressure field.
  - Cons: Tuning of γ

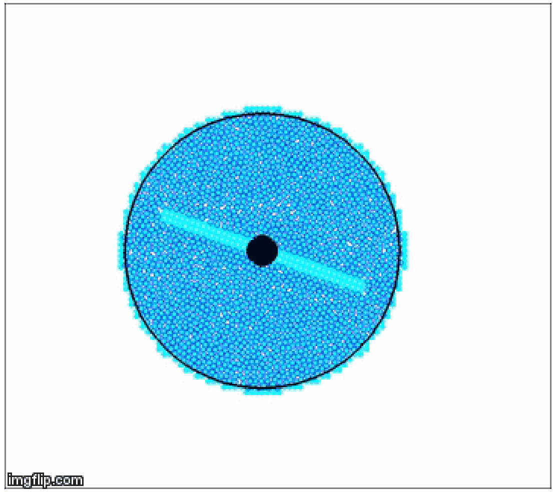
  - Some applications: mixing problem in vessel

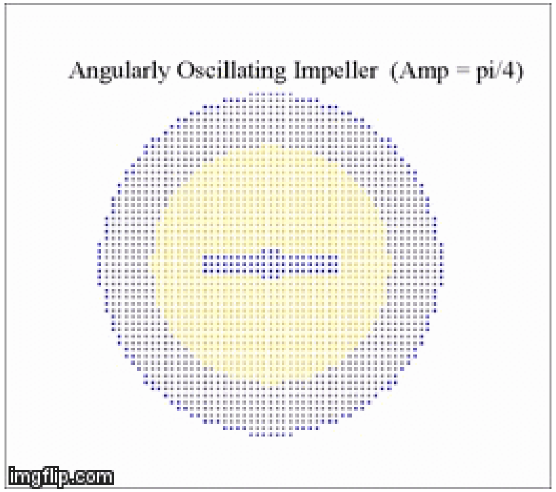
Tanaka, M. and Masunaga, T. (2010), "Stabilization and smoothing of pressure in MPS method by quasi-compressibility", Journal of Computational Physics, Vol. 229, pp. 4279-4290.

Poisson Equation in MPS

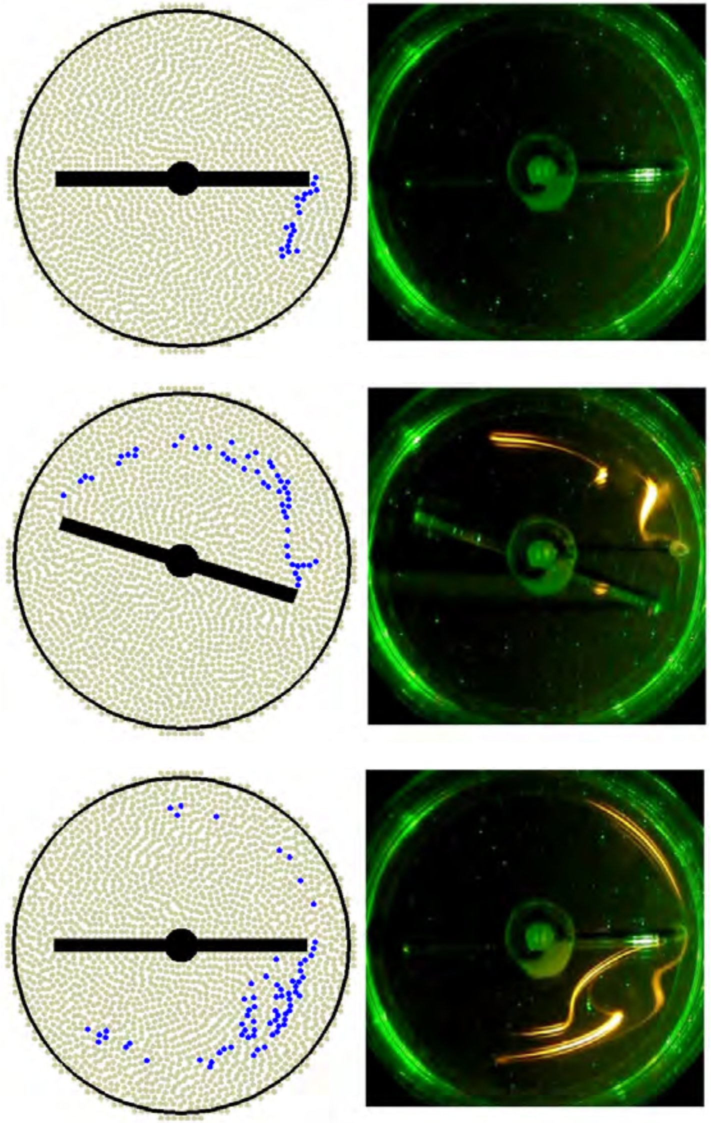
$$\frac{\Delta t}{\rho_i}\nabla^2 P_i^{n+1} = \nabla \bullet \vec{u}_i^{\,*} + \gamma \frac{1}{\Delta t}\frac{n_i^o - n_i^k}{n_i^o}$$

γ must be carefully chosen.





Ng, K.C. and Ng, E.Y.K. (2013), "Laminar mixing performances of baffling, shaft eccentricity and unsteady mixing in a cylindrical vessel", Chemical Engineering Science, Vol. 104, pp. 960-974.



MPS Experiment

streakline

Pressure gradient in MPS

- MPS schemes tend to over-predict the inter-particle attractive forces (causing clumping of particles)
- To solve this problem , an **artificial repulsive force** term is normally incorporated in the MPS pressure gradient model:
  - Minimum pressure model (widely used)

$$\langle \nabla p \rangle_i = \frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_j - p_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2} (\boldsymbol{r}_j - \boldsymbol{r}_i) w(|\boldsymbol{r}_j - \boldsymbol{r}_i|) + \frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_i - \hat{p}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2} (\boldsymbol{r}_j - \boldsymbol{r}_i) w(|\boldsymbol{r}_j - \boldsymbol{r}_i|)$$

Actual MPS gradient model

Ref: Koshizuka, S. and Oka, Y. (1996), "Moving-Particle Semi-implicit method for fragmentation of incompressible fluid", Nuclear Science and Engineering, Vol. 123, pp. 421-434.

Pressure gradient in MPS

- CMPS method (Khayyer and Gotoh 2008):

$$\langle \nabla p \rangle_i = \frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_j - p_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2} (\boldsymbol{r}_j - \boldsymbol{r}_i) w(|\boldsymbol{r}_j - \boldsymbol{r}_i|)$$

Actual MPS gradient model

$$+ \frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_i - \hat{p}_i) + (p_i - \hat{p}_j)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2} (\boldsymbol{r}_j - \boldsymbol{r}_i) w(|\boldsymbol{r}_j - \boldsymbol{r}_i|)$$

Artificial repulsive force

- It is important to note that artificial repulsive force term is not physical by nature.

Khayyer, A. and Gotoh, H. (2008), “Development of CMPS method for accurate water-surface tracking in breaking waves”, Coastal Engineering Journal, Vol. 50, No. 2, pp. 179-207.

The emergence of MPPM

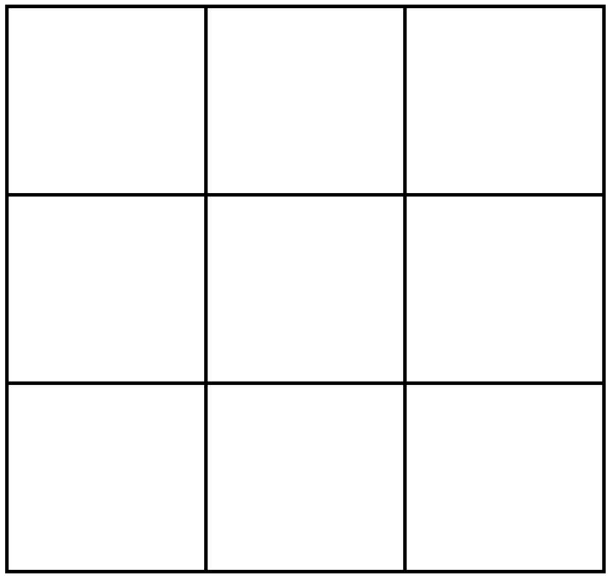
- Designed to tackle the noisy pressure field of MPS.
- Velocity? Solved on Particle Level (Lagrangian)
- Pressure? Solved on Mesh Level (Eulerian). Pressure is not a convective variable. → Ensure local divergence-free condition!!
- "Divergence-free" PPE is written on local mesh P.

$$\frac{\Delta t}{\rho_P} \nabla^2 P_P^{n+1} = \nabla \bullet \vec{u}_P^{\,*}$$

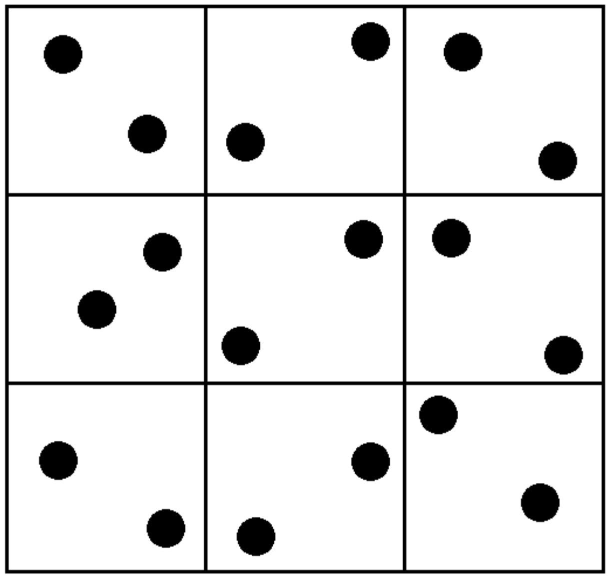
- Strength:
  - Coefficient of PPE is built only once. Save time.
  - Tuning-free for pressure gradient!

Hwang, Y.H. (2011), "A moving particle method with embedded pressure mesh (MPPM) for incompressible flow calculations", Numerical Heat Transfer, Part B, Vol. 60, pp. 370-398.

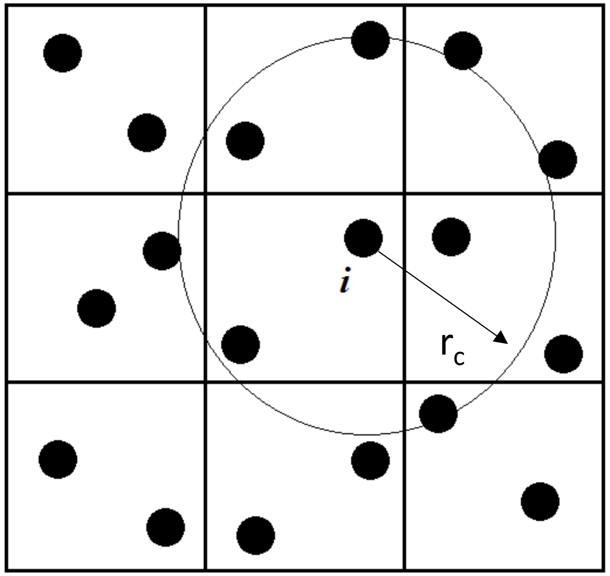
MPPM Step 1:Background mesh of flow problem



MPPM Step 2: Particle at time level n.

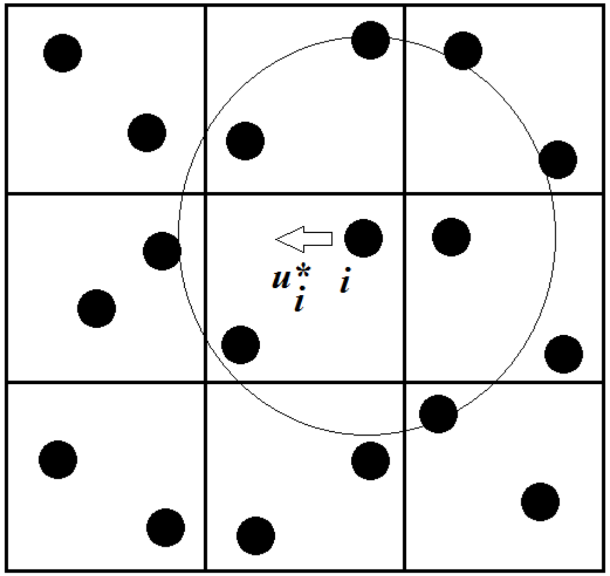


MPPM Step 3: Laplacian velocity



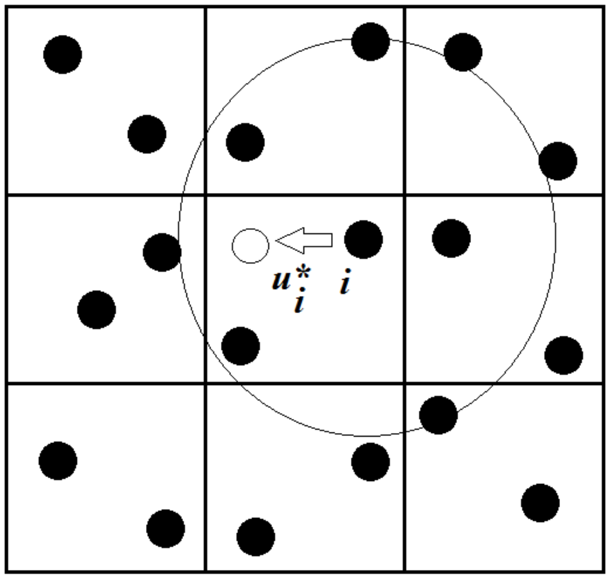
$$\mu_i \nabla^2 (\vec{u})_i^n$$

MPPM Step 4: Particle velocity at time *



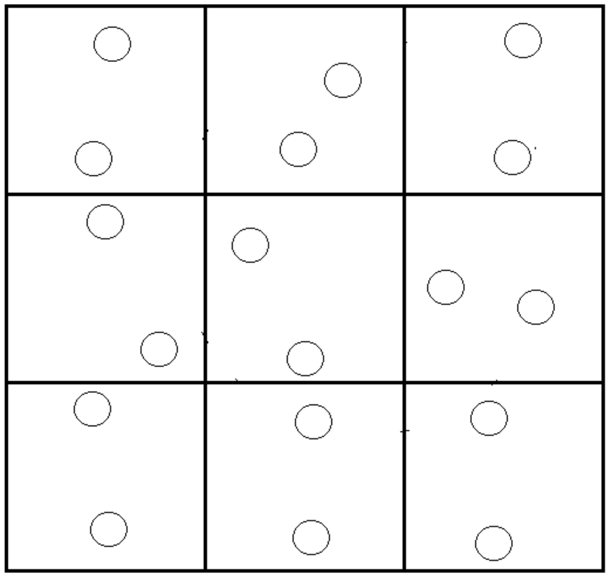
$$\vec{u}_i^* = \vec{u}_i^n + \frac{\Delta t}{\rho_i}\left(\mu_i \nabla^2 (\vec{u})_i^n + \vec{S}_i^n\right)$$

MPPM Step 5: Particle position at time *

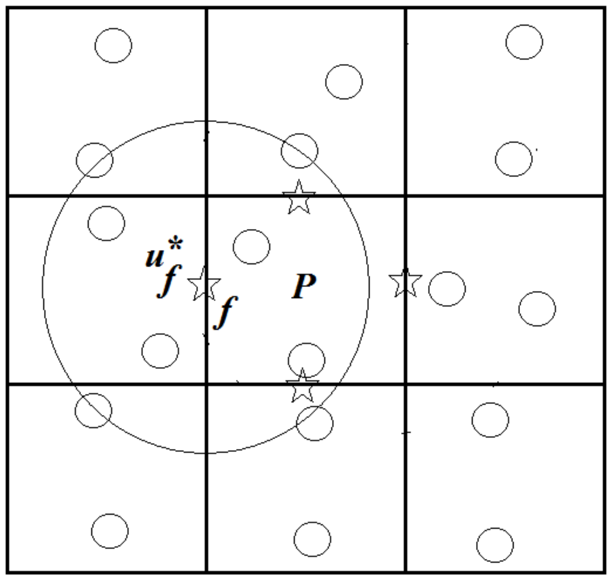


$$\vec{r}_i^{\,*} = \vec{r}_i^{\,n} + \Delta t \vec{u}_i^{\,*}$$

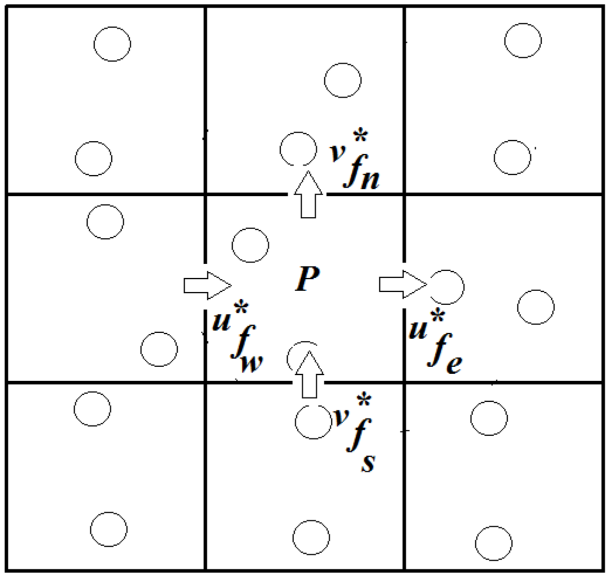
MPPM Step 6: All particle positions at time *



MPPM Step 7: Mesh face velocity at time *

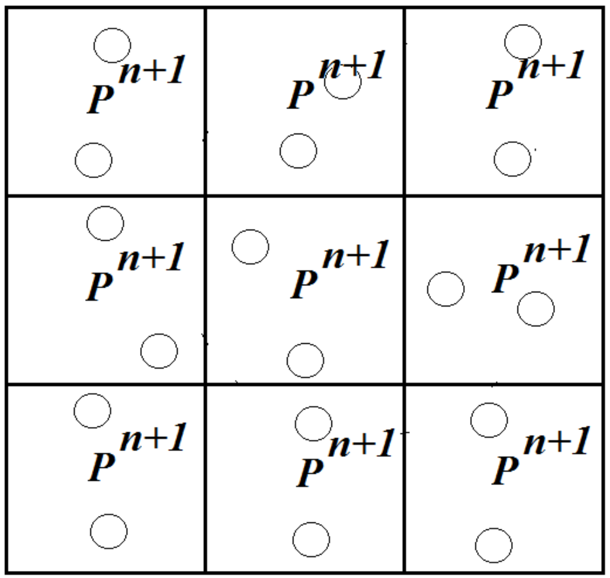


MPPM Step 8: Poisson Equation of Pressure

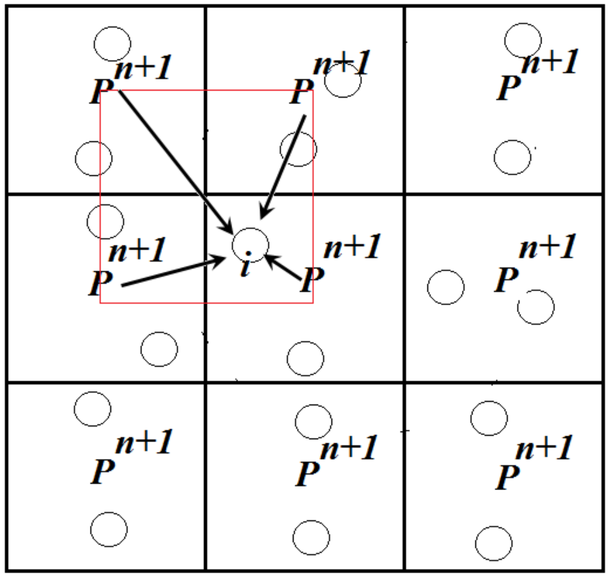


$$\frac{\Delta t}{\rho_P}\nabla^2 P_P^{n+1} = \nabla \bullet \vec{u}_P^*$$

MPPM Step 9: Updated mesh pressure P^{n+1}

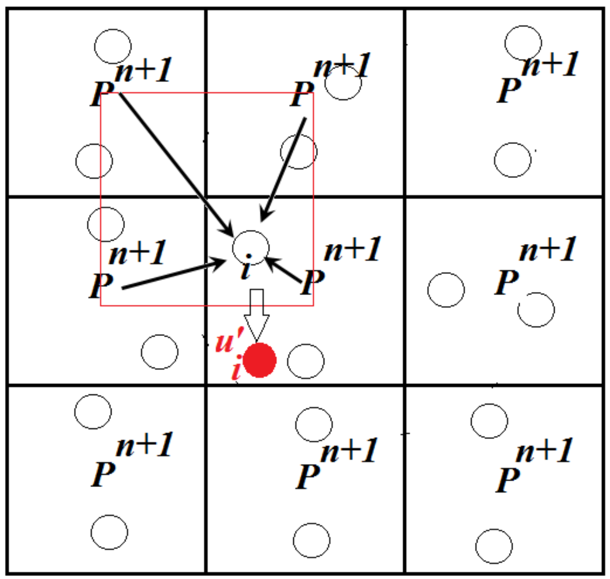


MPPM Step 10: Pressure Gradient at particle *i*



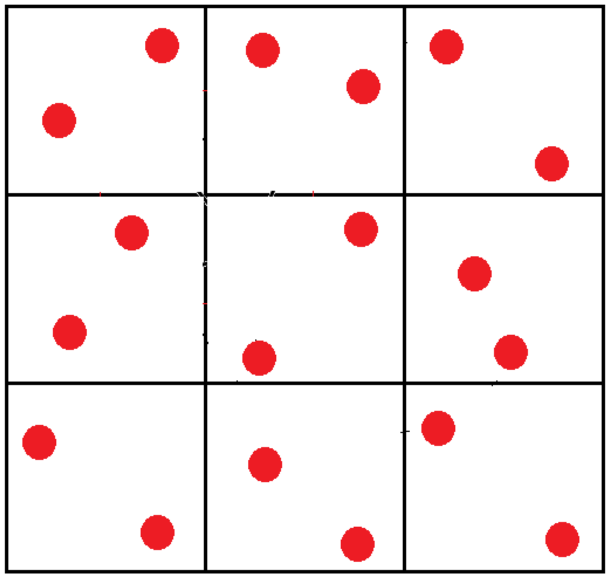
- Via bi-linear interpolation, etc.

MPPM Step 11: Velocity correction



$$\vec{u}_i' = -\frac{\Delta t}{\rho_i}\nabla P_i^{n+1}$$

MPPM Step 12: Correct velocity and positions



$$\vec{u}_i^{n+1} = \vec{u}_i^{*} + \vec{u}_i^{'}$$

$$\vec{r}_i^{n+1} = \vec{r}_i^{n} + \Delta t \vec{u}_i^{n+1}$$

Roles of Particle and Mesh in MPPM

- Background mesh:
  - PPE
  - Particle searching

- Particles
  - Tackle convective term (via Lagrangian)
  - As observation points (no volume property)
  - Particle penetrating from wall? Delete it.
  - Not enough particle within a region? Add it.

Some drawbacks in conventional MPPM

- Background grid is Cartesian based. Simple geometry.
- Laplacian operator of MPS is used:

$$\nabla^2(\vec{u})_i^n = \frac{2d}{\sum_{j\neq i} w\left(\left|\vec{r}_j - \vec{r}_i\right|\right)\left|\vec{r}_j - \vec{r}_i\right|^2} \sum_{j\neq i} w\left(\left|\vec{r}_j - \vec{r}_i\right|\right)\left(\vec{u}_j^n - \vec{u}_i^n\right)$$

  - Modified Equation: Inconsistent for irregular particle layout (Hwang et al. 2016)
- Explicit marching – limited time step size (stability)

YH Hwang, KC Ng, TWH Sheu (2016), "An improved particle smoothing procedure for Laplacian operator in a randomly scattered cloud" Numerical Heat Transfer, Part B: Fundamentals, 2016

UMPPM: consistency in Laplacian

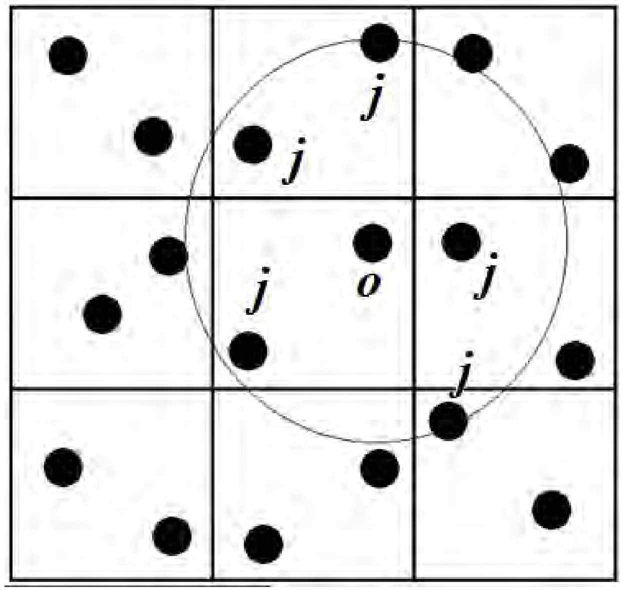
- Generalized Finite Difference (GFD) of *Koh et al. (2012).*

$$f(x,y) = f_0 + hf_{,x0} + kf_{,y0} + \frac{1}{2}h^2 f_{,xx0} + hkf_{,xy0} + \frac{1}{2}k^2 f_{,yy0} + O(r^3),$$

$$[\mathbf{A}]\{D\mathbf{f}\} - \{\mathbf{f}\} = 0$$

$$[\mathbf{A}] = \begin{bmatrix} h_1 & k_1 & \frac{1}{2}h_1^2 & h_1k_1 & \frac{1}{2}k_1^2 \\ h_2 & k_2 & \frac{1}{2}h_2^2 & h_2k_2 & \frac{1}{2}k_2^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ h_N & k_N & \frac{1}{2}h_N^2 & h_Nk_N & \frac{1}{2}k_N^2 \end{bmatrix}$$

$$\{D\mathbf{f}\} = \begin{Bmatrix} f_{,x0} \\ f_{,y0} \\ f_{,xx0} \\ f_{,xy0} \\ f_{,yy0} \end{Bmatrix}, \qquad \{\mathbf{f}\} = \begin{Bmatrix} f_1 - f_0 \\ f_2 - f_0 \\ \vdots \\ f_N - f_0 \end{Bmatrix},$$



Koh, C.G., Gao, M. and Luo, C. (2012), "A new particle method for simulation of incompressible free surface flow problems", International Journal for Numerical Methods in Engineering, Vol. 89, pp. 1582-1604.

UMPPM: consistency in Laplacian

- Least square error E and minimizing:

$$\|\mathbf{E}\| = \sum_{j=1}^{N} \left[f_0 - f_j + h_j f_{,x0} + k_j f_{,y0} + 0.5 h_j^2 f_{,xx0} + h_j k_j f_{,xy0} + 0.5 k_j^2 f_{,yy0} \right]^2 w_j^2,$$

$$\frac{\partial \|\mathbf{E}\|}{\partial \{D\mathbf{f}\}} = 0$$

$$\begin{bmatrix} a_1 & a_2 & a_3 & a_4 & a_5 \\ b_1 & b_2 & b_3 & b_4 & b_5 \\ c_1 & c_2 & c_3 & c_4 & c_5 \\ d_1 & d_2 & d_3 & d_4 & d_5 \\ e_1 & e_2 & e_3 & e_4 & e_5 \end{bmatrix}^{-1} \begin{Bmatrix} f_{,x0} \\ f_{,y0} \\ f_{,xx0} \\ f_{,xy0} \\ f_{,yy0} \end{Bmatrix} = \begin{pmatrix} \sum f_j w_j^2 h_j - f_0 \sum w_j^2 h_j \\ \sum f_j w_j^2 k_j - f_0 \sum w_j^2 k_j \\ \sum f_j w_j^2 \frac{h_j^2}{2} - f_0 \sum w_j^2 \frac{h_j^2}{2} \\ \sum f_j w_j^2 h_j k_j - f_0 \sum w_j^2 h_j k_j \\ \sum f_j w_j^2 \frac{k_j^2}{2} - f_0 \sum w_j^2 \frac{k_j^2}{2} \end{pmatrix}$$

UMPPM: consistency in Laplacian

- Coefficients *a, b, c, d, e* (Koh et al. 2013)

$$
\begin{bmatrix} a_1 & a_2 & a_3 & a_4 & a_5 \\ b_1 & b_2 & b_3 & b_4 & b_5 \\ c_1 & c_2 & c_3 & c_4 & c_5 \\ d_1 & d_2 & d_3 & d_4 & d_5 \\ e_1 & e_2 & e_3 & e_4 & e_5 \end{bmatrix} = \begin{bmatrix}
\sum_{j\neq i} w_j^2 h_j^2 & \sum_{j\neq i} w_j^2 h_j k_j & 0.5\sum_{j\neq i} w_j^2 h_j^3 & \sum_{j\neq i} w_j^2 h_j^2 k_j & 0.5\sum_{j\neq i} w_j^2 h_j k_j^2 \\
\sum_{j\neq i} w_j^2 h_j k_j & \sum_{j\neq i} w_j^2 k_j^2 & 0.5\sum_{j\neq i} w_j^2 h_j^2 k_j & \sum_{j\neq i} w_j^2 h_j k_j^2 & 0.5\sum_{j\neq i} w_j^2 k_j^3 \\
0.5\sum_{j\neq i} w_j^2 h_j^3 & 0.5\sum_{j\neq i} w_j^2 h_j^2 k_j & 0.25\sum_{j\neq i} w_j^2 h_j^4 & 0.5\sum_{j\neq i} w_j^2 h_j^3 k_j & 0.25\sum_{j\neq i} w_j^2 h_j^2 k_j^2 \\
\sum_{j\neq i} w_j^2 h_j^2 k_j & \sum_{j\neq i} w_j^2 h_j k_j^2 & 0.5\sum_{j\neq i} w_j^2 h_j^3 k_j & \sum_{j\neq i} w_j^2 h_j^2 k_j^2 & 0.5\sum_{j\neq i} w_j^2 h_j k_j^3 \\
0.5\sum_{j\neq i} w_j^2 h_j k_j^2 & 0.5\sum_{j\neq i} w_j^2 k_j^3 & 0.25\sum_{j\neq i} w_j^2 h_j^2 k_j^2 & 0.5\sum_{j\neq i} w_j^2 h_j k_j^3 & 0.25\sum_{j\neq i} w_j^2 k_j^4
\end{bmatrix}^{-1}
$$

Koh, C.G., Luo, M., Gao, M. and Bai, W. (2013), "Modelling of liquid sloshing with constrained floating baffle", Computers and Structures, Vol. 122, pp. 270-279.

UMPPM: Implicitness

- We solve the Laplacian of *u* and *T* implicitly.

$$\nabla^2(\vec{u})_i^* = (\vec{u})_{xx}^* + (\vec{u})_{yy}^*$$

$$= \sum_{j \neq i} w_j^{\,2} \left[(c_1+e_1)h_j + (c_2+e_2)k_j + (c_3+e_3)\frac{h_j^{\,2}}{2} + (c_4+e_4)h_j k_j + (c_5+e_5)\frac{k_j^{\,2}}{2} \right] \left(\vec{u}_j^{\,*} - \vec{u}_i^{\,*} \right)$$

$$\nabla^2(T)_i^* = (T)_{xx}^* + (T)_{yy}^*$$

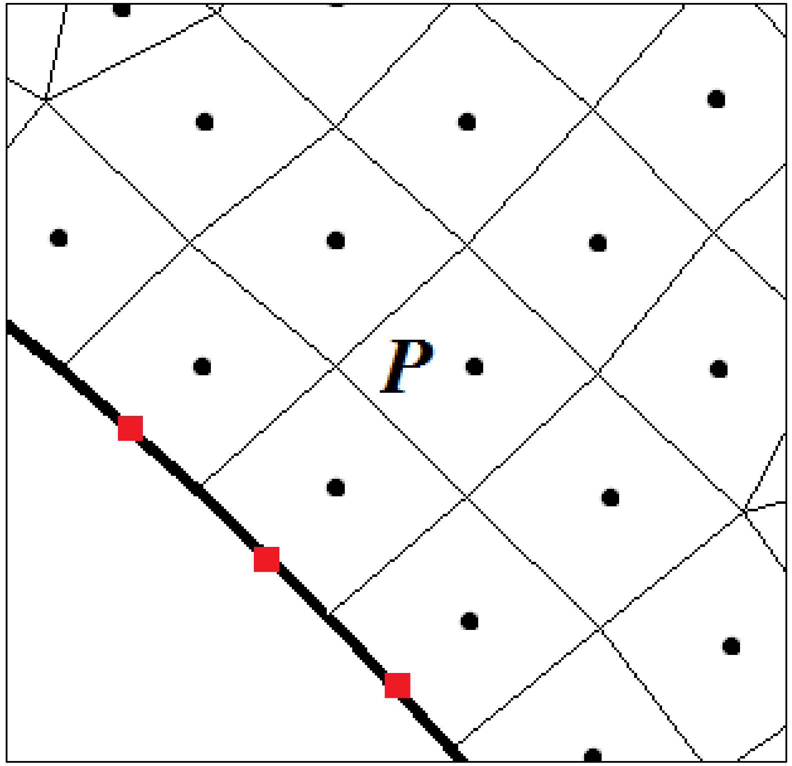
$$= \sum_{j \neq i} w_j^{\,2} \left[(c_1+e_1)h_j + (c_2+e_2)k_j + (c_3+e_3)\frac{h_j^{\,2}}{2} + (c_4+e_4)h_j k_j + (c_5+e_5)\frac{k_j^{\,2}}{2} \right] \left(T_j^* - T_i^* \right)$$

UMPPM: unstructured pressure mesh

- Address <u>complex geometry problem.</u>
- Use of body-fitted unstructured mesh.
- PPE in its volume integral form

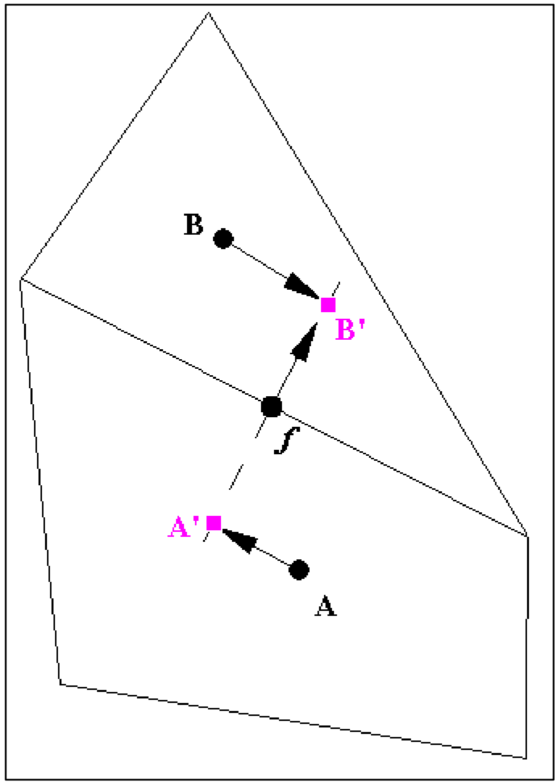
$$\int \nabla^2 P_P^{n+1} dV = \int \frac{\rho_P}{\Delta t} \nabla \bullet \vec{u}_P^* dV$$

$$\sum_f \nabla P_f^{n+1} \bullet \vec{A}_f = \frac{\rho_P}{\Delta t} \sum_f \vec{u}_f^* \bullet \vec{A}_f$$



UMPPM: unstructured pressure mesh

- Handling of mesh non-orthogonality



$$\nabla P_f^{n+1} \bullet \vec{A}_f = \frac{P_{B'}^{n+1} - P_{A'}^{n+1}}{\left\| \overrightarrow{A'B'} \right\|} \left\| \vec{A}_f \right\|$$

$$P_{A'}^{n+1} = P_A^{n+1} + \nabla P_A^{n+1} \bullet \overrightarrow{AA'}$$

$$P_{B'}^{n+1} = P_B^{n+1} + \nabla P_B^{n+1} \bullet \overrightarrow{BB'}$$

UMPPM: unstructured pressure mesh

- Complete PPE for unstructured mesh.

Non-orthogonal correction

$$\sum_f \frac{P_B^{n+1} - P_A^{n+1} + \left[\nabla P_B^{n+1} \bullet \overrightarrow{BB'} - \nabla P_A^{n+1} \bullet \overrightarrow{AA'} \right]}{\left\| \overrightarrow{A'B'} \right\|} \left\| \vec{A}_f \right\| = \frac{\rho_P}{\Delta t} \sum_f \vec{u}_f^{\,*} \bullet \vec{A}_f$$

- The coefficients of PPE are built once. Only source terms are updated at every time step.
- [.] term is zero for orthogonal mesh

Test Case 1: Taylor-Green

Re = 100

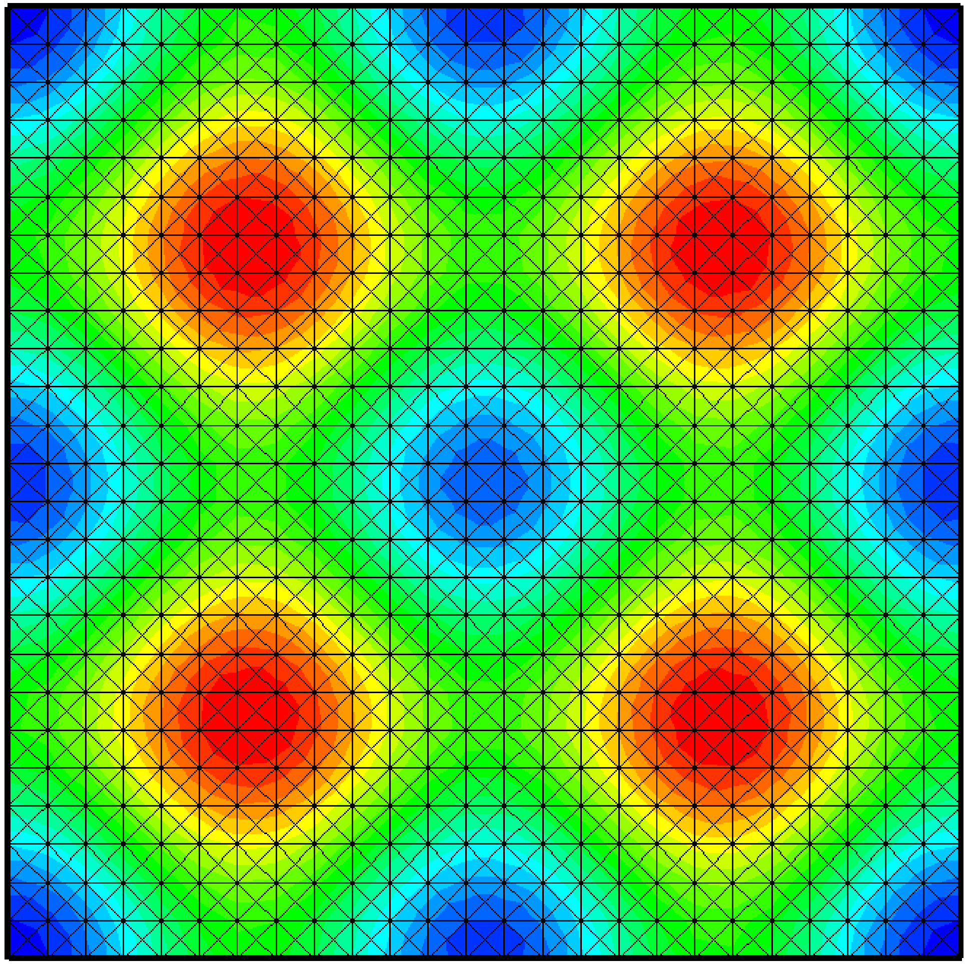
Analytical solution:

$$u_{theo}(x,y,t) = -Ue^{bt}\cos(2\pi x)\sin(2\pi y)$$

$$v_{theo}(x,y,t) = Ue^{bt}\sin(2\pi x)\cos(2\pi y)$$

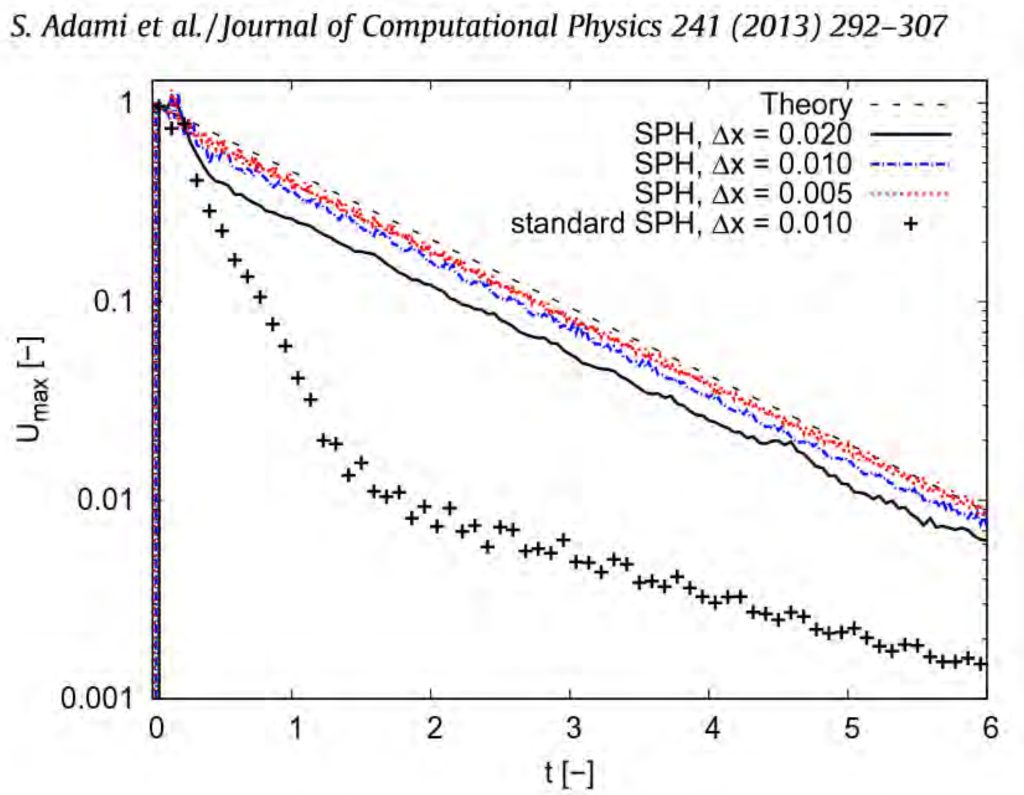
$$P_{theo}(x,y,t) = -\frac{U^2}{4}e^{2bt}\left(\cos(4\pi x)+\cos(4\pi y)\right)$$

- 0 < x, y < 1
- Periodic in all boundaries
- 0 < t < 5 (CFL = 0.25)

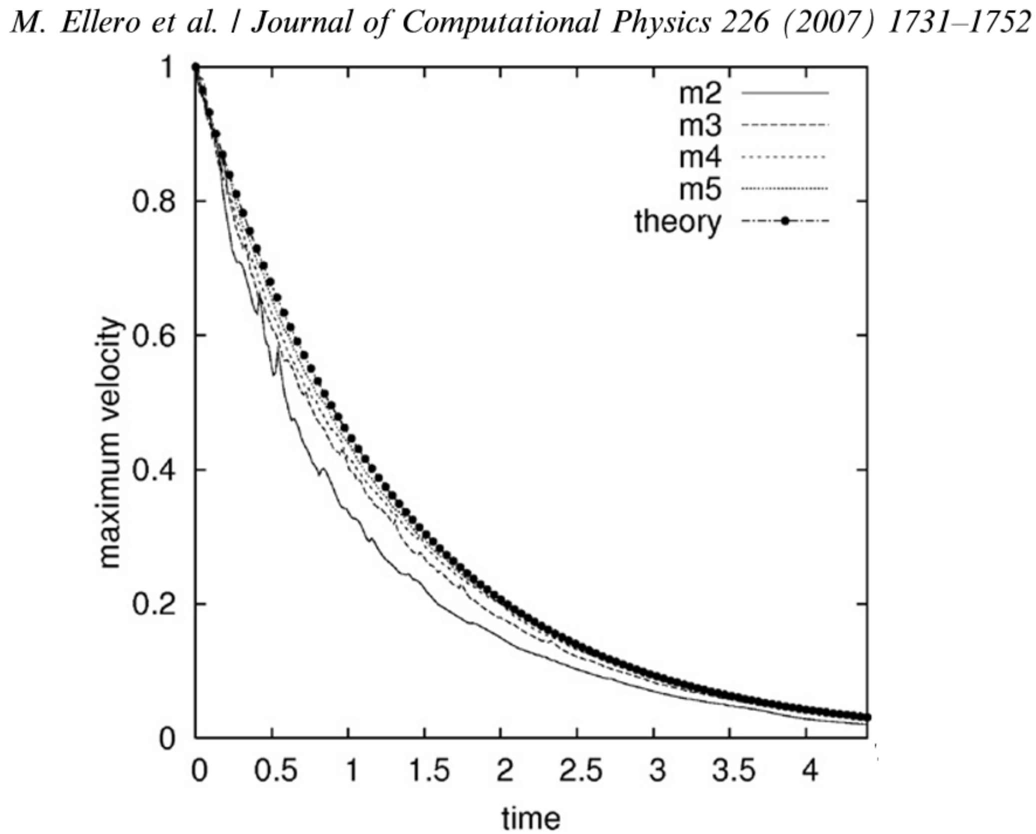


Pressure field (UMPPM)

Comparison of U_{max} vs time (SPH)

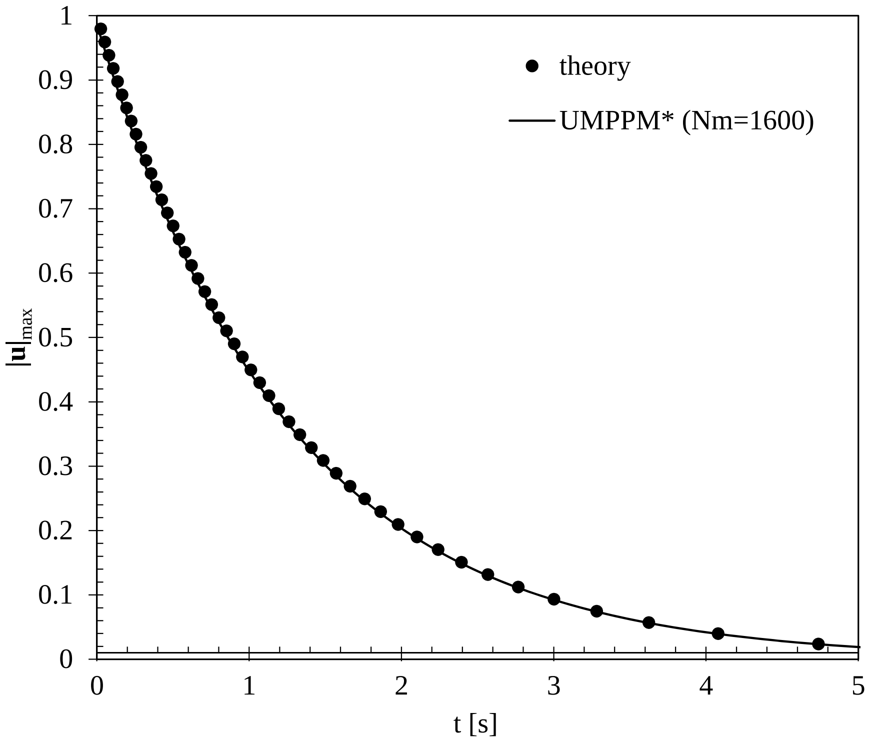


WCSPH: Particle number 2500-40000



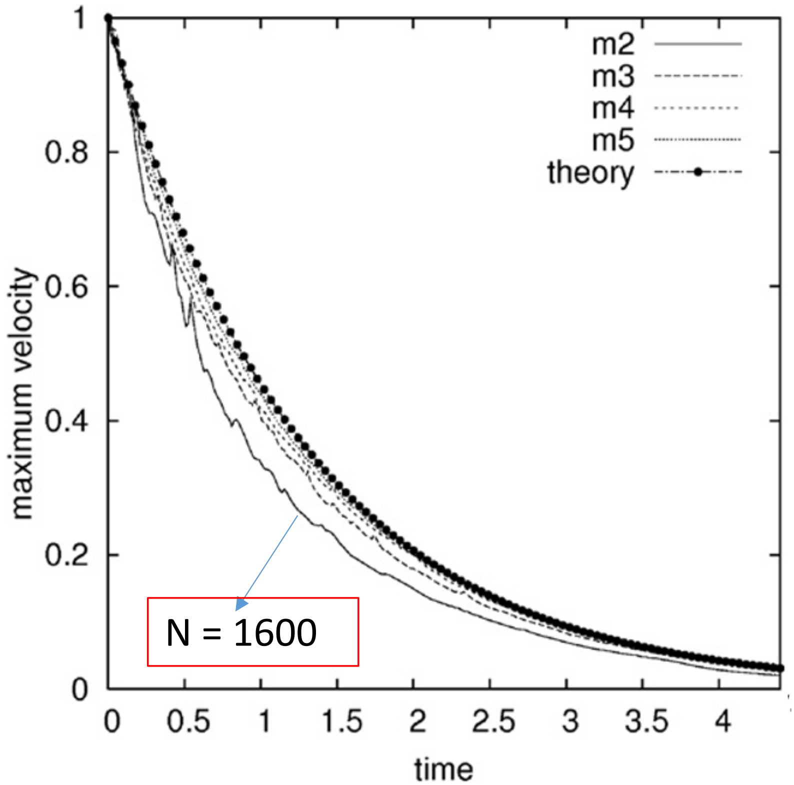
ISPH: Particle number 1600-10000

Comparison of U_{max} vs time (UMPPM)



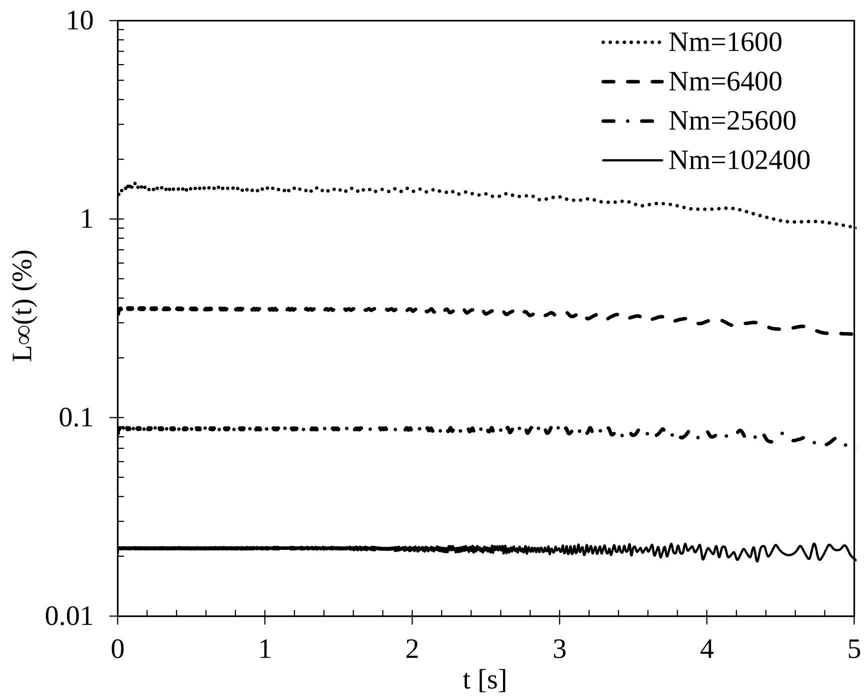
N = 1600

M. Ellero et al. / Journal of Computational Physics 226 (2007) 1731–1752

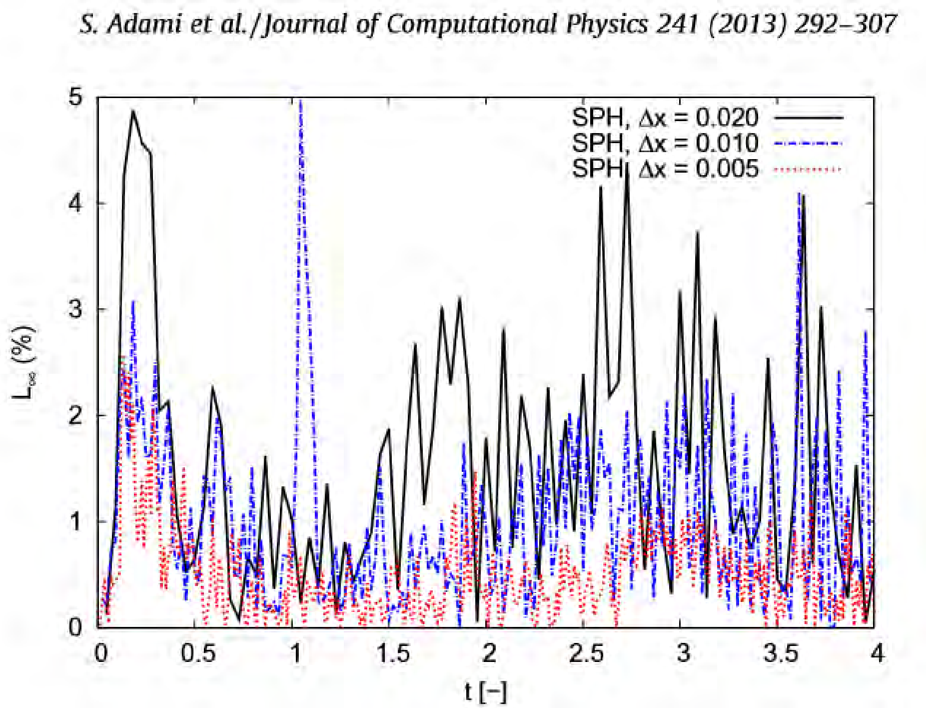


ISPH: Particle number 1600-10000

Measurement of $L_\infty(t) = \frac{|\max\|\vec{u}_P\| - Ue^{bt}|}{Ue^{bt}}$

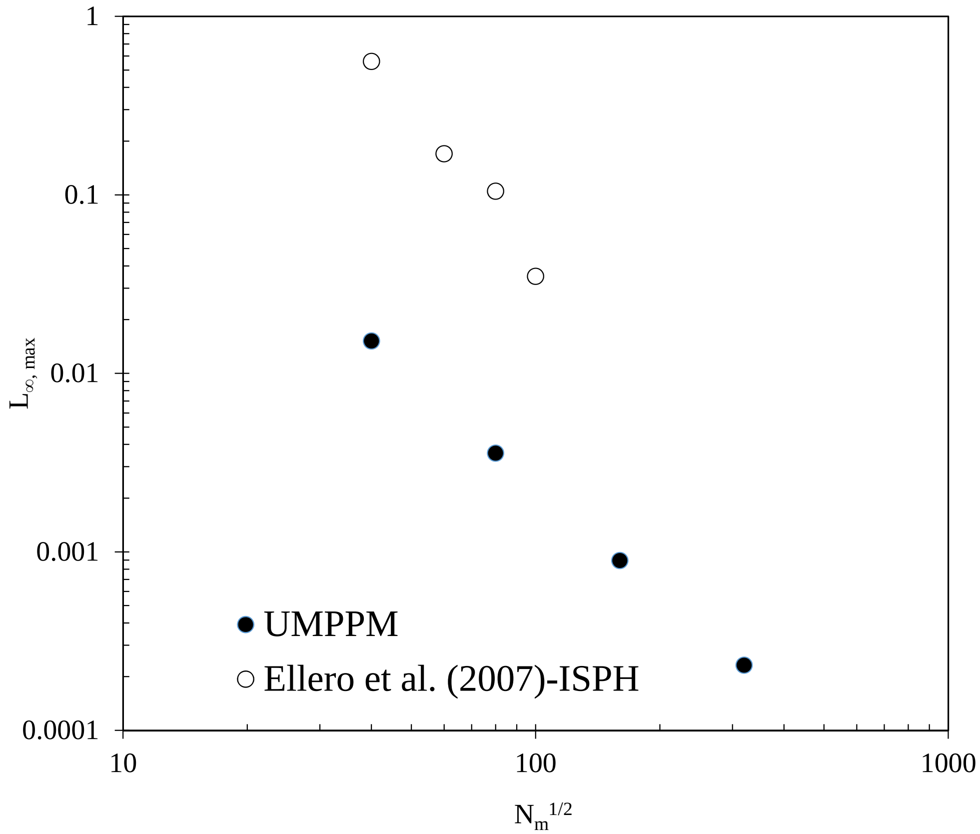


UMPPM

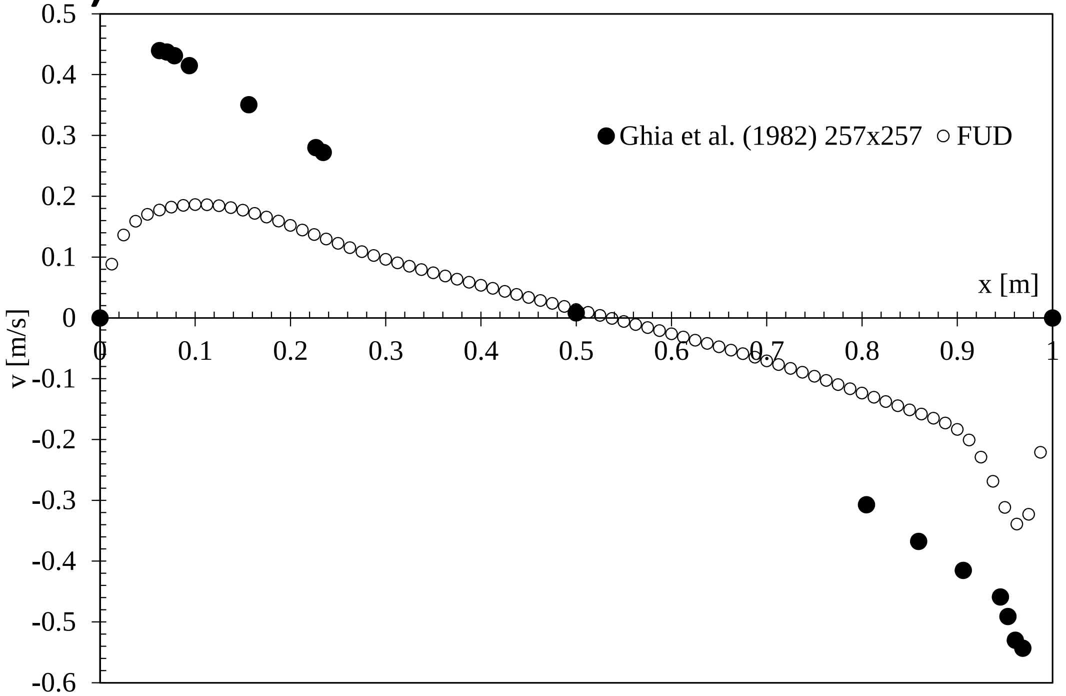


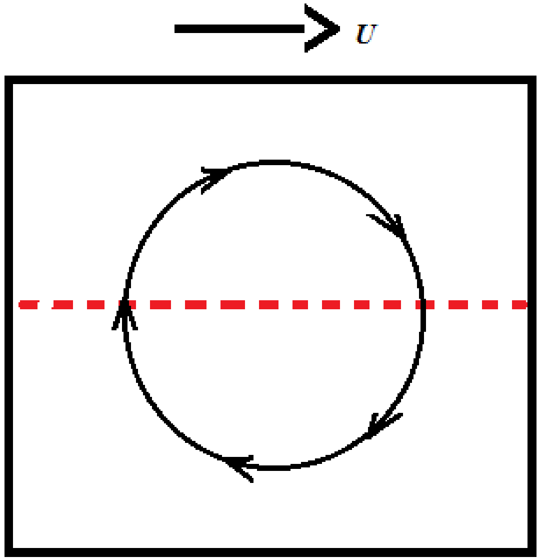
WCSPH: Particle number 2500-40000

Comparison of $L_{\infty,max}$



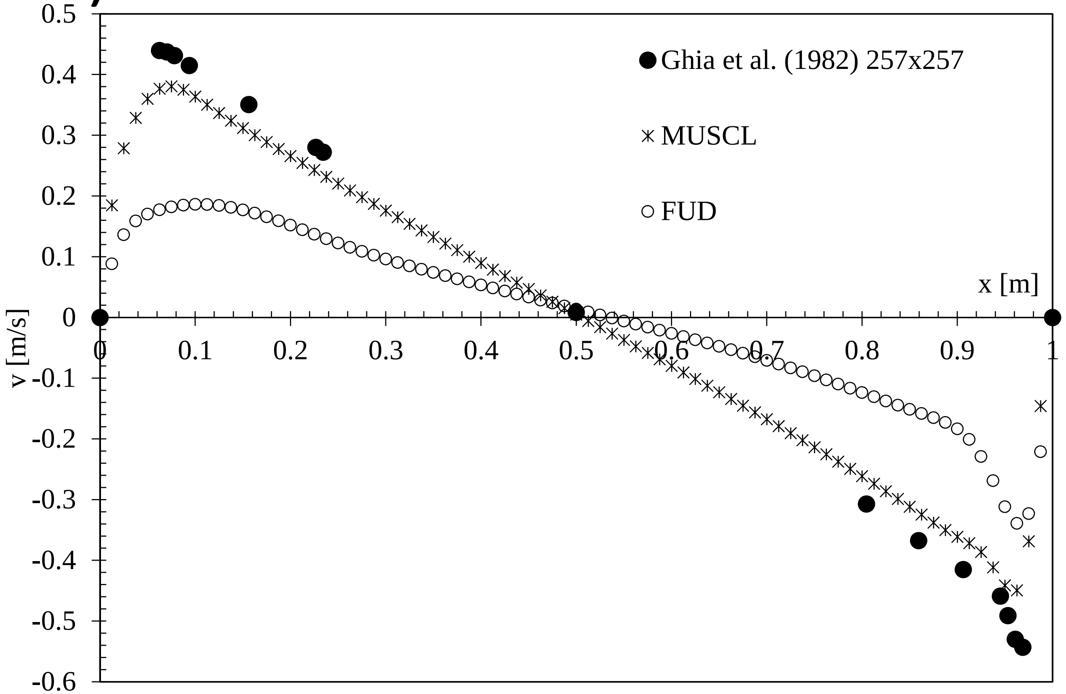
Test Case 2: Lid-driven flow in square cavity (Re = 10000)

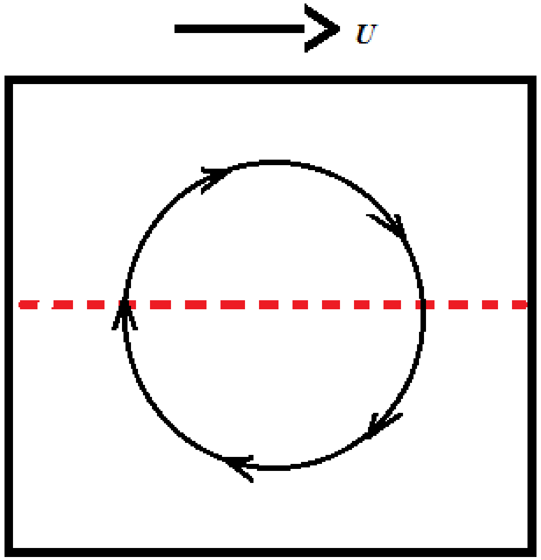




- First-order Upwind (FLUENT)- (80x80 mesh)

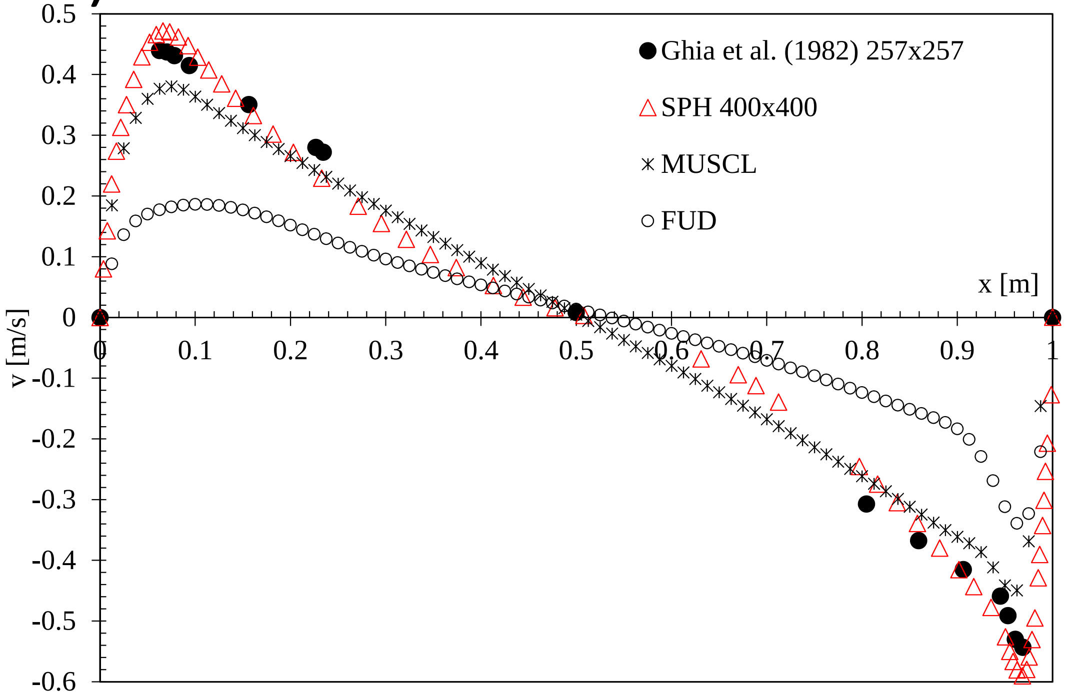
Verification: Lid-driven flow in square cavity (Re = 10000)

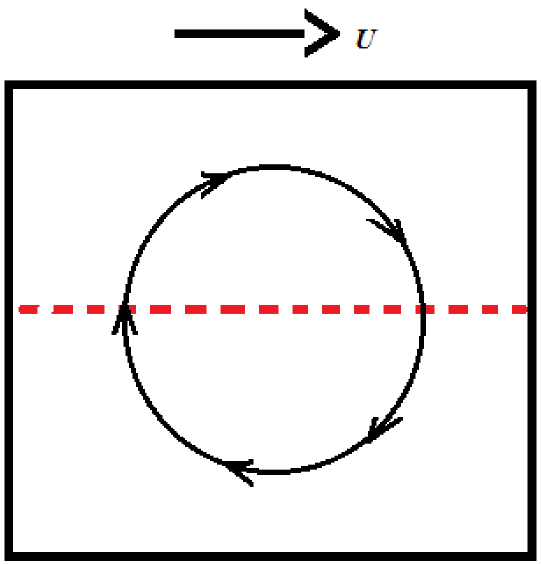




- 3rd-order MUSCL (FLUENT)- (80x80 mesh)

Verification: Lid-driven flow in square cavity (Re = 10000)

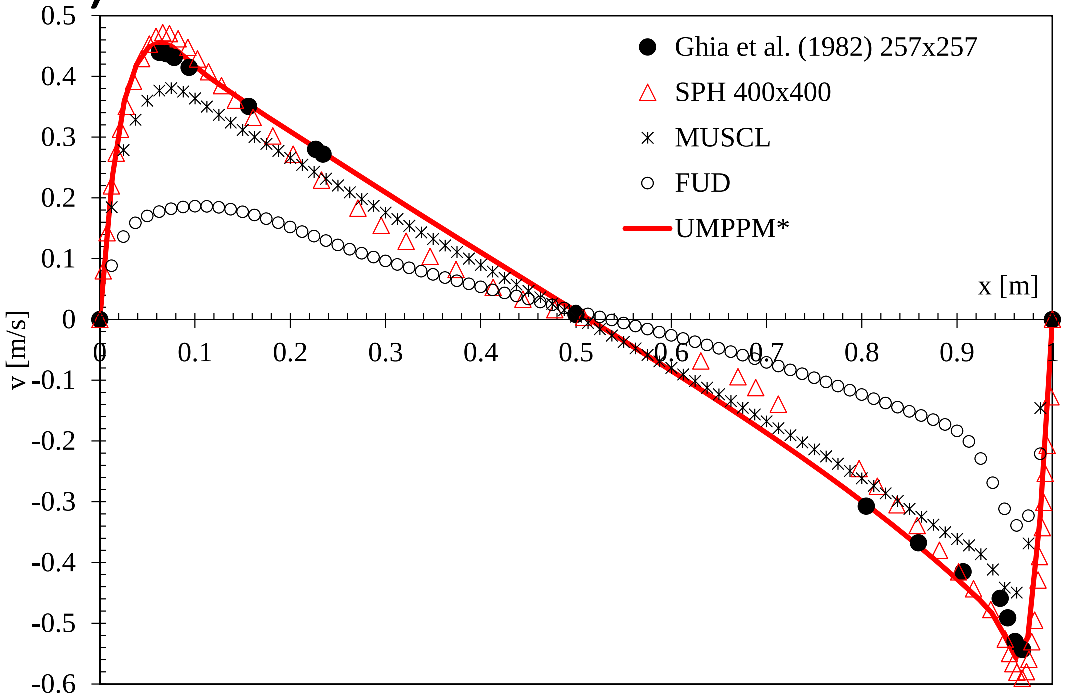


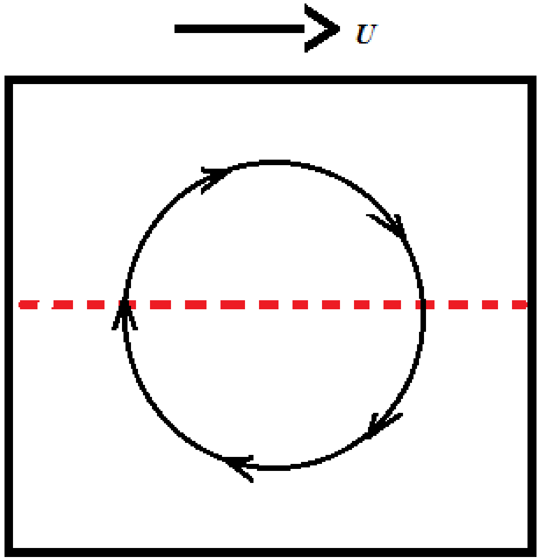


- SPH (400x400) – Adami et al. (2013)

Adami, S., Hu, X.Y. and Adams, N.A. (2013), "A transport-velocity formulation for smoothed particle hydrodynamics", Journal of Computational Physics, Vol. 241, pp. 292-307.

Verification: Lid-driven flow in square cavity (Re = 10000)

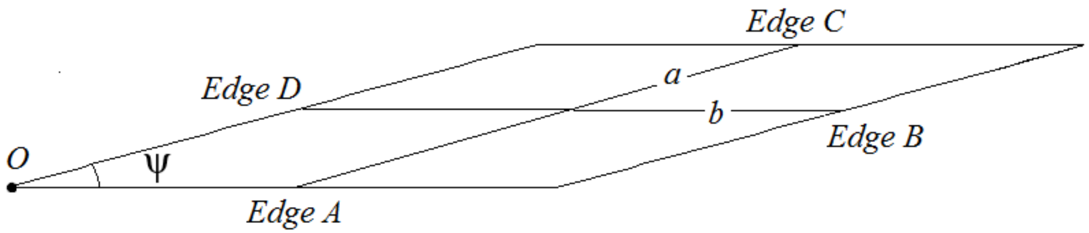


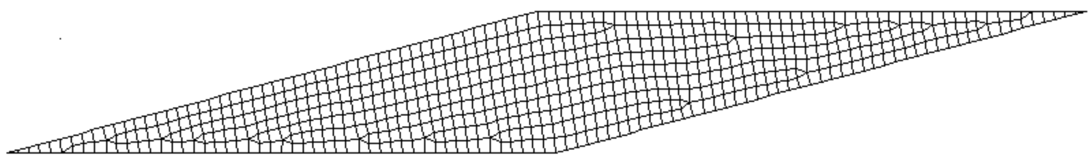


- UMPPM (80x80 mesh) ~ 15,000 particles at statistically steady state.

Test case 3: Lid-driven flow in skewed cavity (Re = 1000)

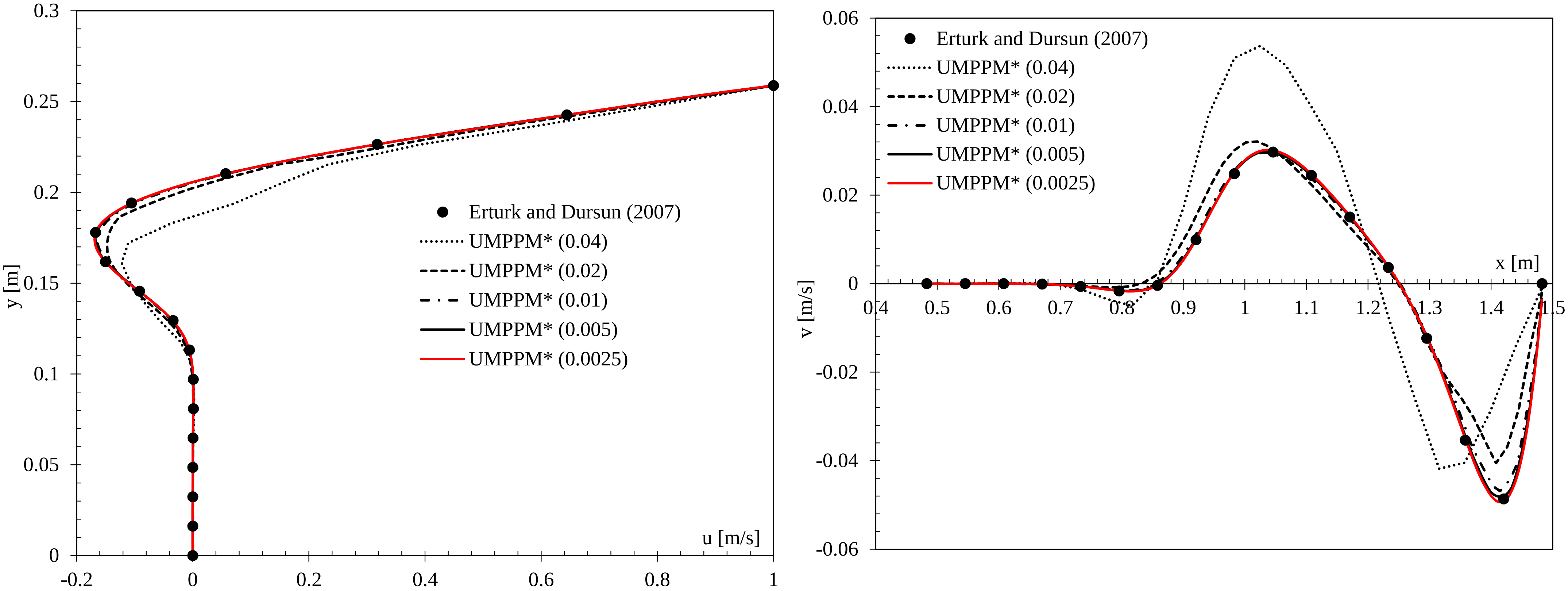
- Length = 1.0m



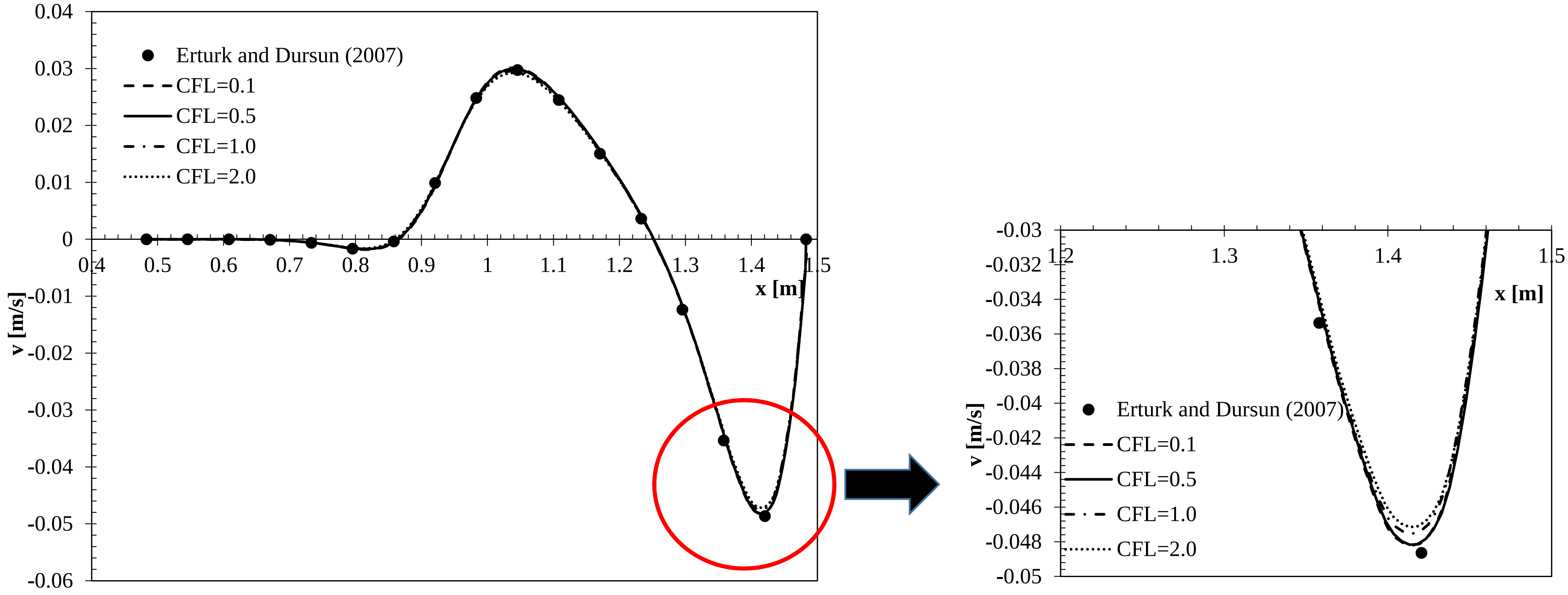


Erturk, E. and Dursun, B. (2007), "Numerical solutions of 2D steady incompressible flow in a driven skewed cavity", ZAMM-Journal of Applied Mathematics and Mechanics, Vol. 87, pp. 377-392.

Convergence Test

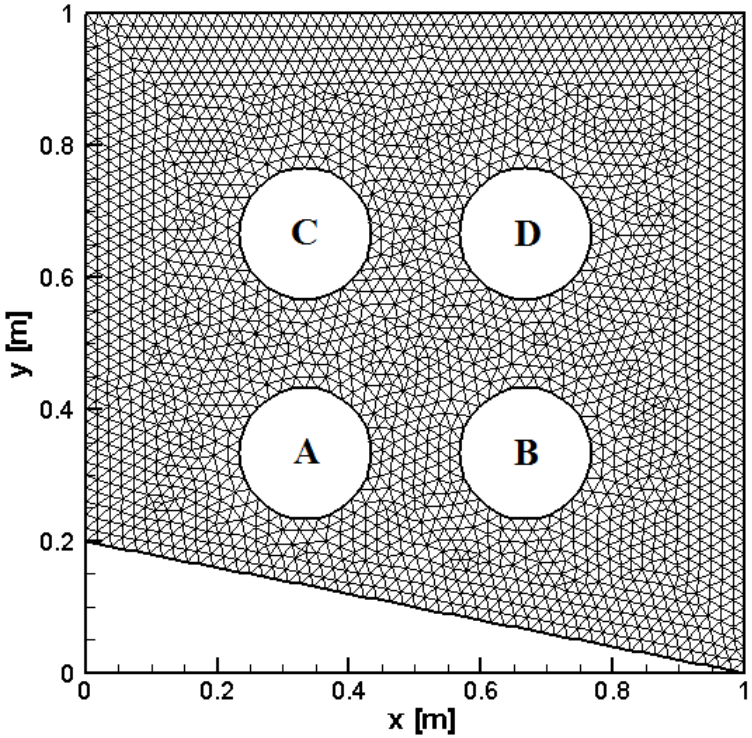


Effect of CFL



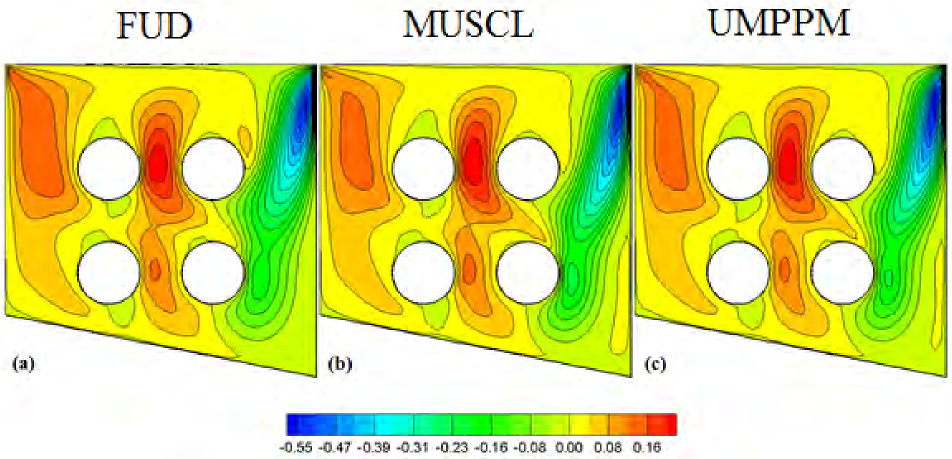
Test case 4: Lid-driven flow in complex cavity

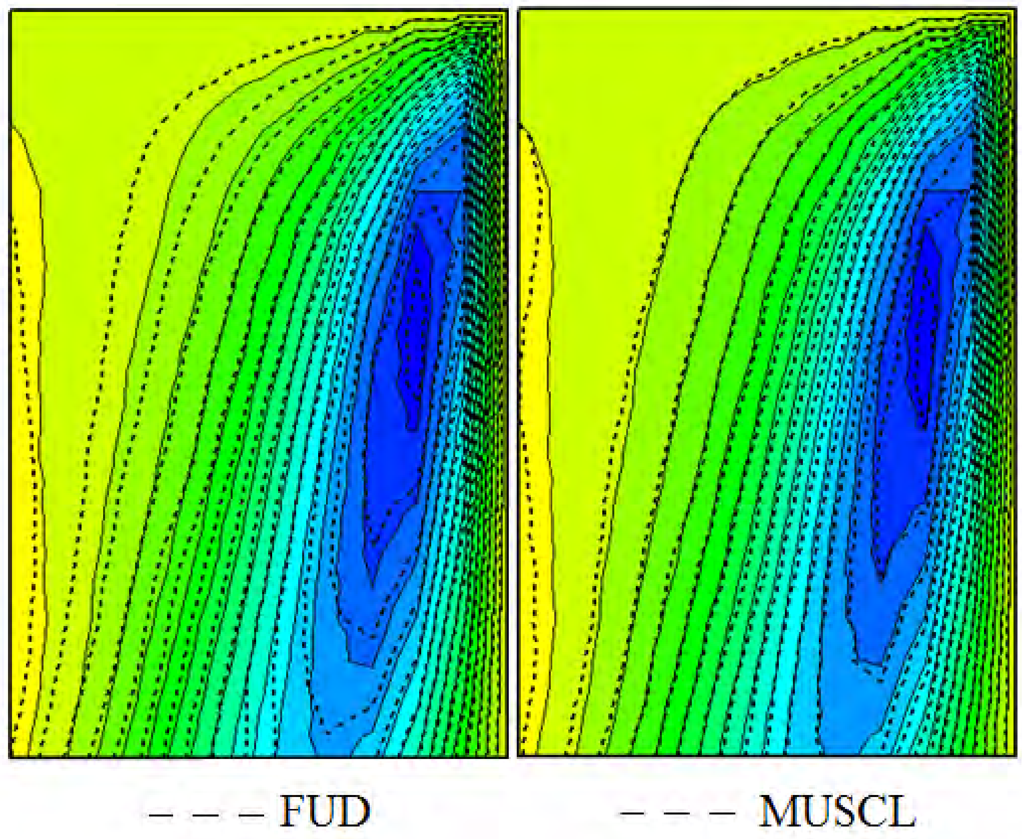
- Re = 1000



Comparison with FLUENT

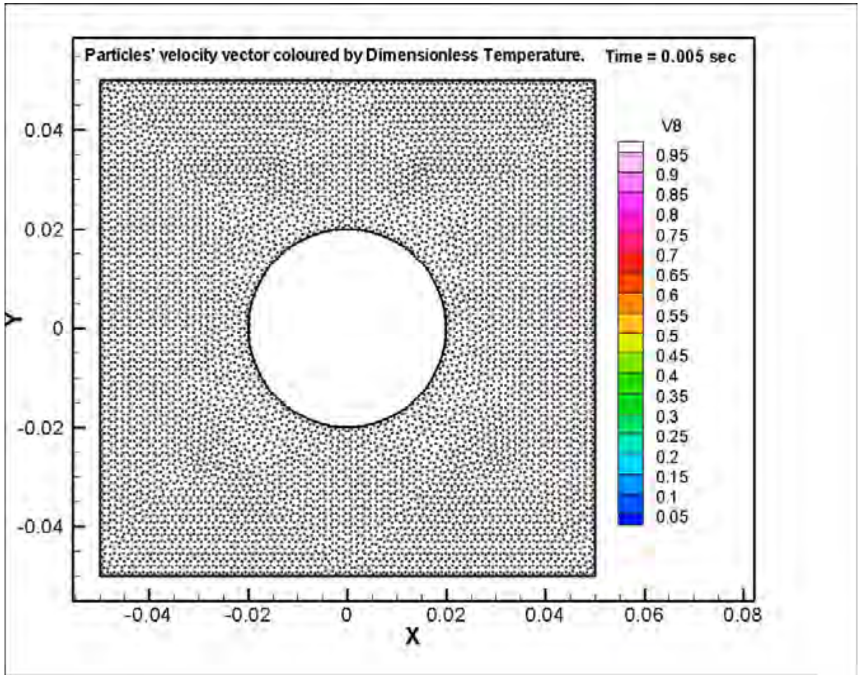
- Y-velocity





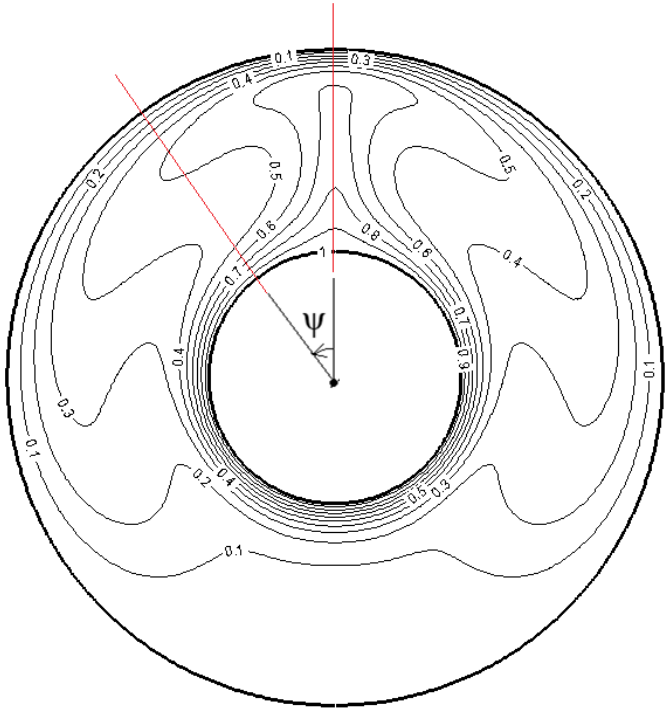
Test case 5: Natural convection

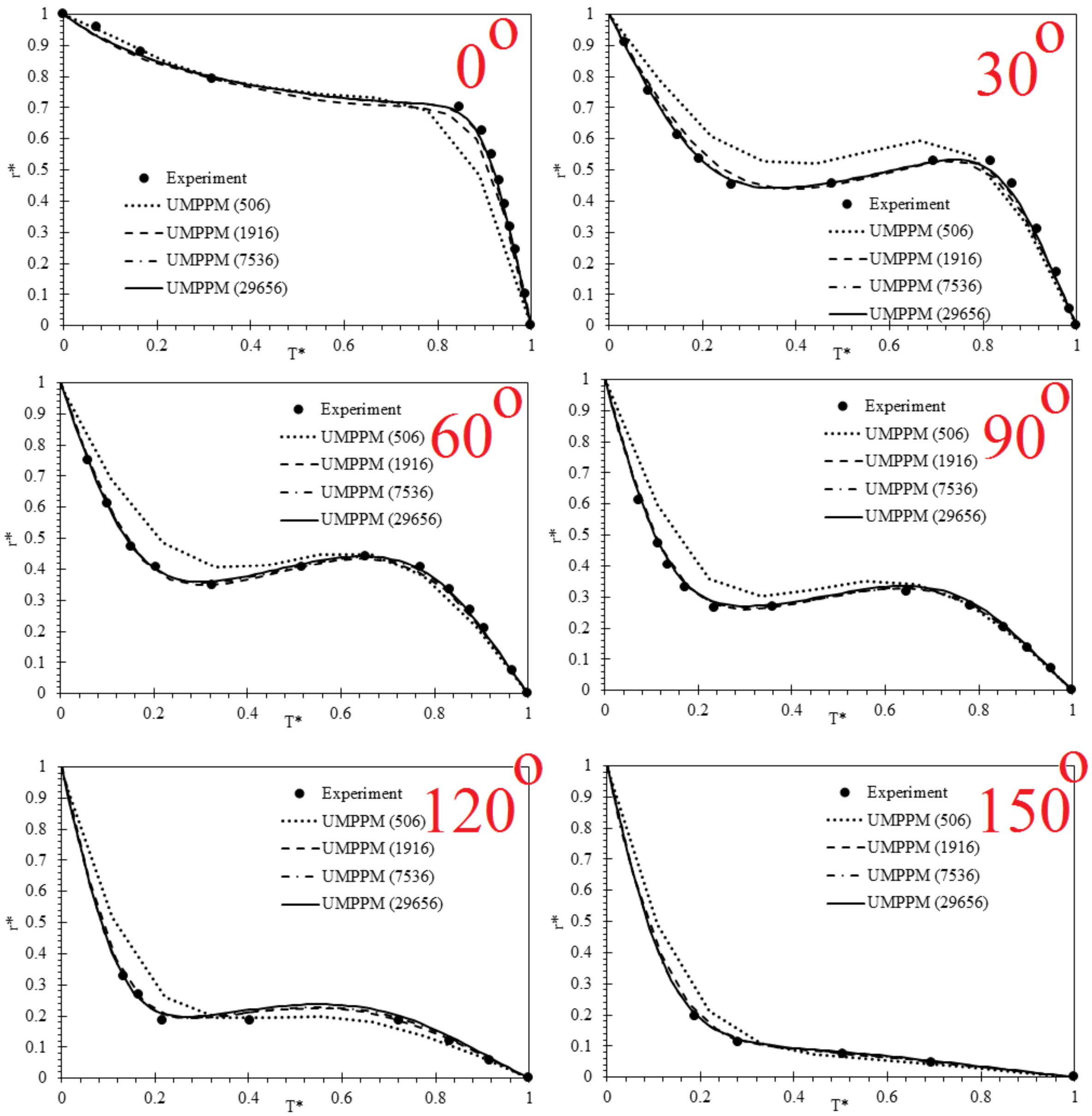
- T_{inner} = 323.664K
- T_{outer} = 300K
- C_p = 1006 J/kgK
- k = 0.02816 W/mK
- Ra = 97600 (same as exp. Kuehn et al 1976)



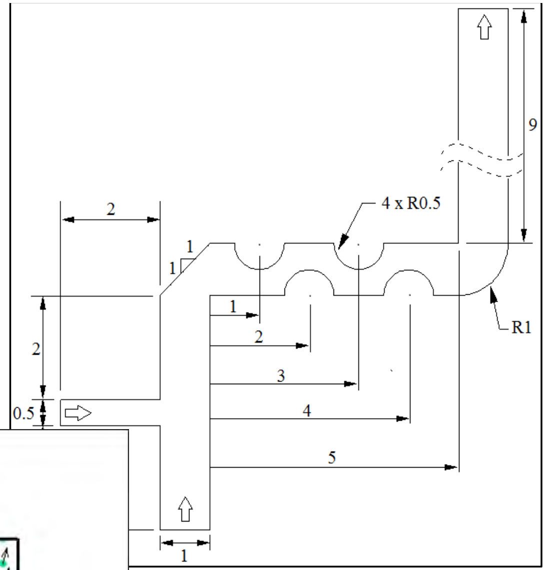
Validation

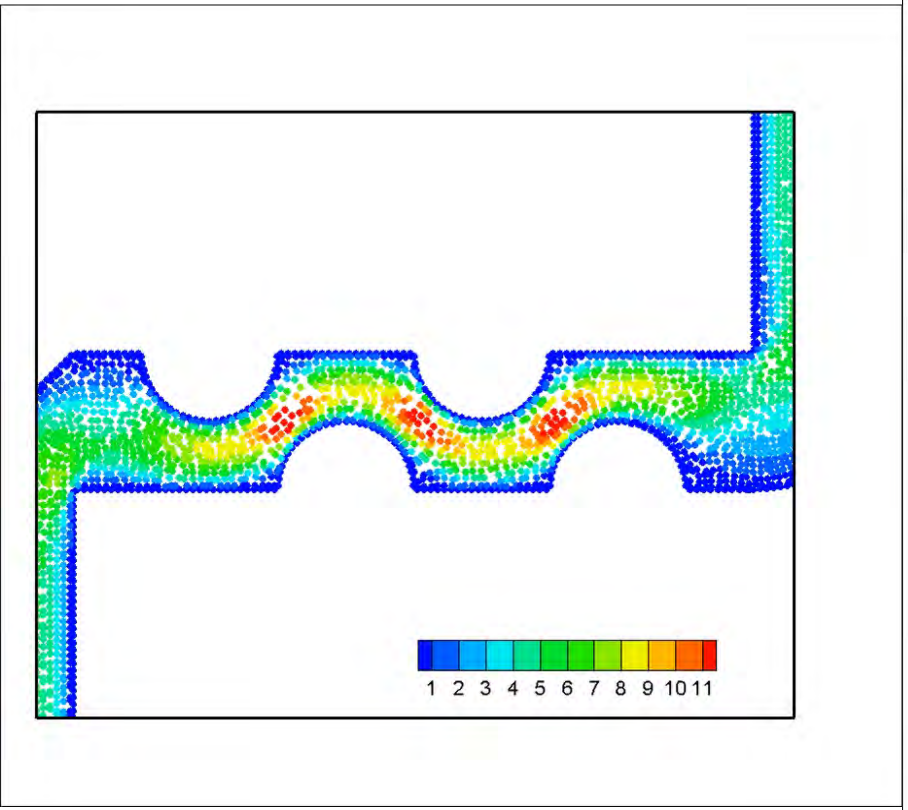
- Temperature (spatial convergence)

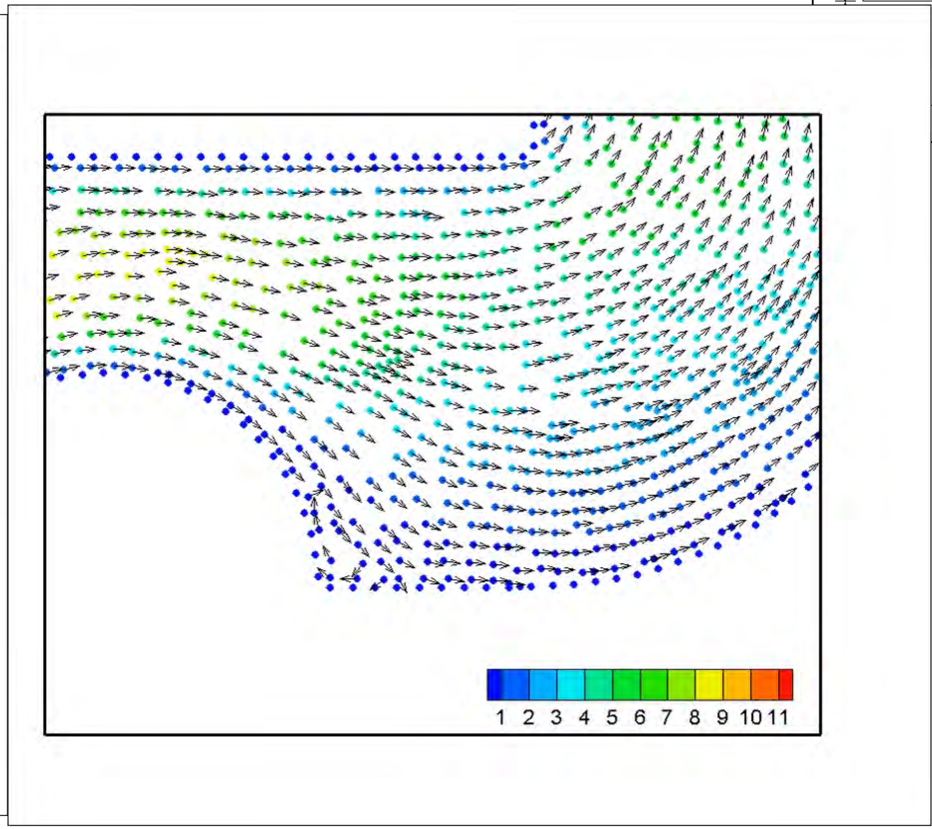




Test case 6: Flow in complex channel

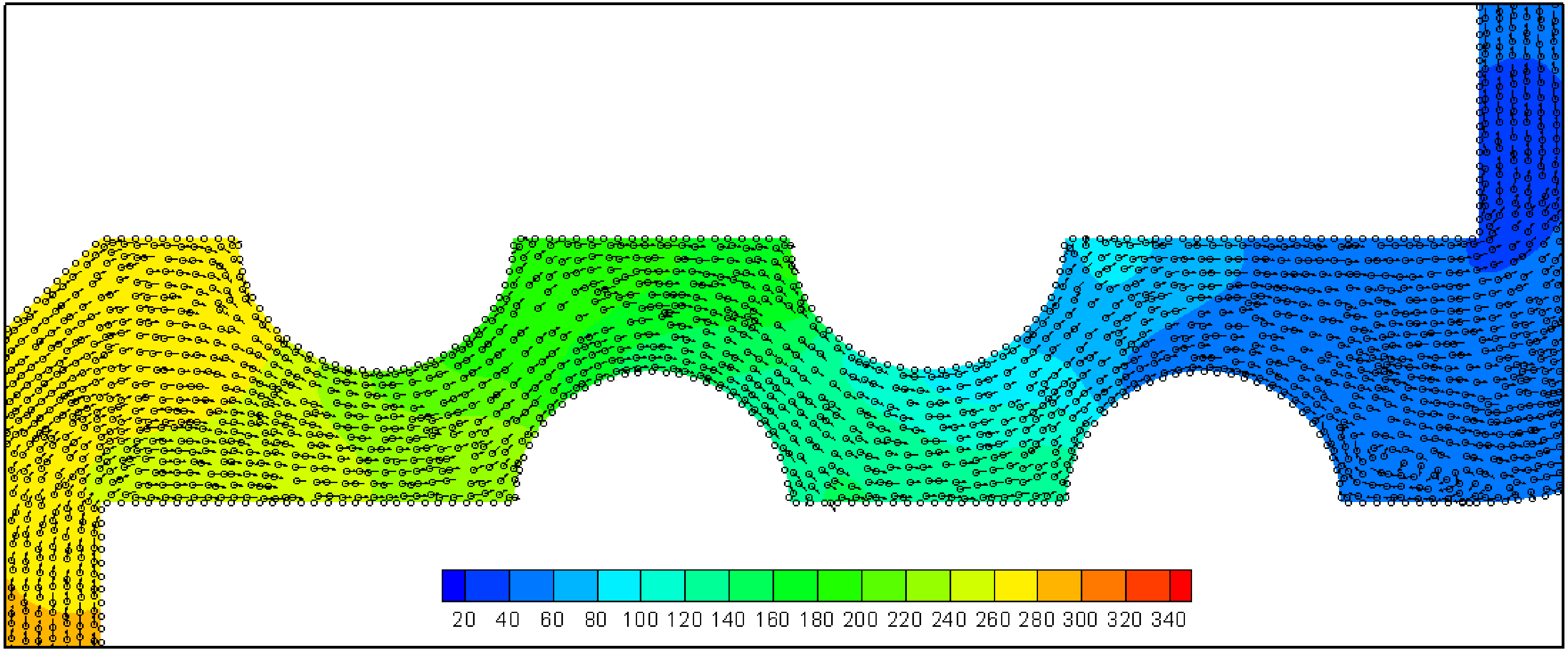






Test case 6: Flow in complex channel

- Pressure field



Conclusion

- UMPPM is able to address the limitations of current MPPM in
  - Complex domain (unstructured mesh)
  - Time step constraint (implicit method)
  - Inconsistent Laplacian (GFD)
- Results of UMPPM exhibits numerical consistency in Taylor-Green vortex decay problem.
- Stable even CFL > 1.0 (=2.0)
- Use of unstructured mesh is robust. Can handle various engineering-related problems.

Thank you for your attention!

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Unstructured Moving Particle Pressure Mesh (UMPPM) method for incompressible isothermal and non-isothermal flow computation

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