Modeling of Circulating Fluidized Bed System

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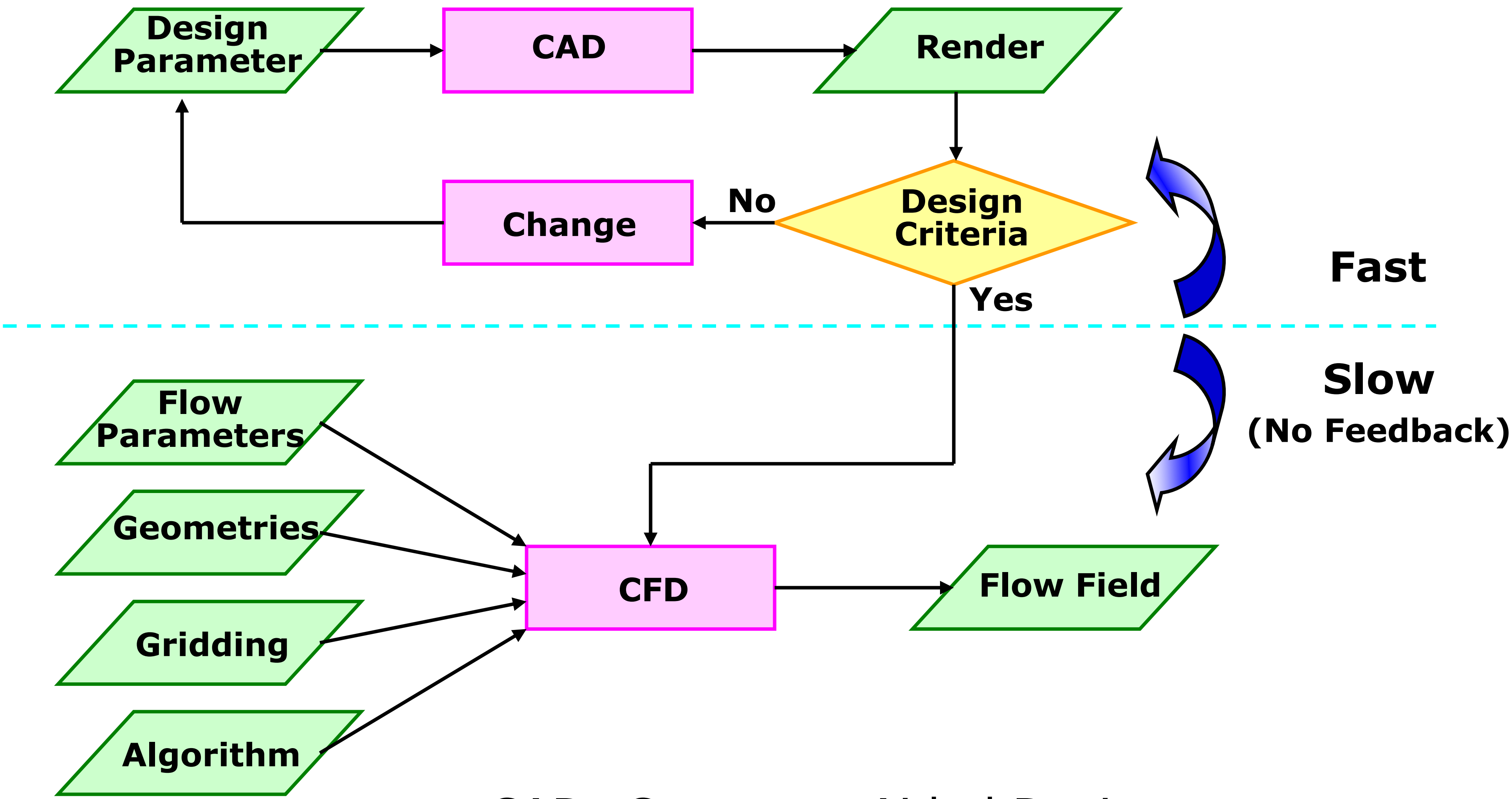
Outline

1. **Introduction**
2. **Fast Network Model (FNM)**
   Case Study I: Hot Gas Filtration (HGF)
   Case Study II: Circulating Fluidized Bed (CFB)
3. **Smoothed Particle Hydrodynamics (SPH)**
   Weakly Compressible Flow
   Vorticity Formulation
4. **Hybridized Computational Fluid Dynamics (CFD) Method & Virtual Reality Demonstration**
5. **Conclusion**

Typical Fluid Design Process



CAD: Computer Aided Design

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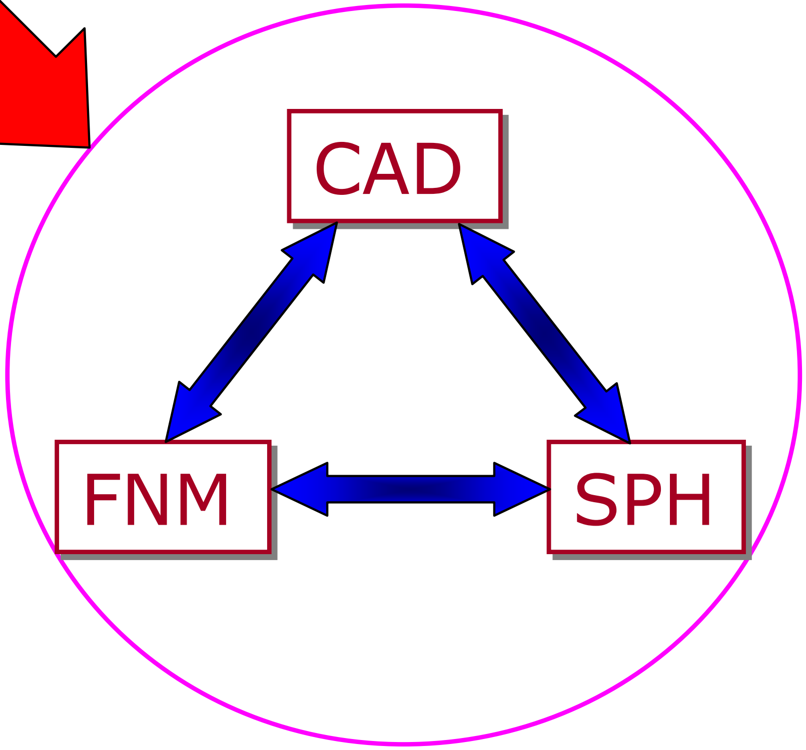
Objectives

The Design of Power Plants

- Various Components
- Geometrically and Aerodynamically Complex
- Difficulties in Conventional CFD Methods
- Need for a Numerically Simple and Fast Model to Couple with CAD



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Strategy

Circulating Fluidized Bed (CFB)

⇕

Multiphase Flow
Turbulence
Chemical Reaction

⇕

Hybridized CFD Method

Hybridized CFD Method

FNM

- Simplest Method
- Sparse Network Nodes
- Fast Simulation Speed

SPH

- Transient
- Gridless
- Easily Parallelizable
- Easy to Hybridize

Couple through Pseudo-particles

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Fast Network Model (FNM)

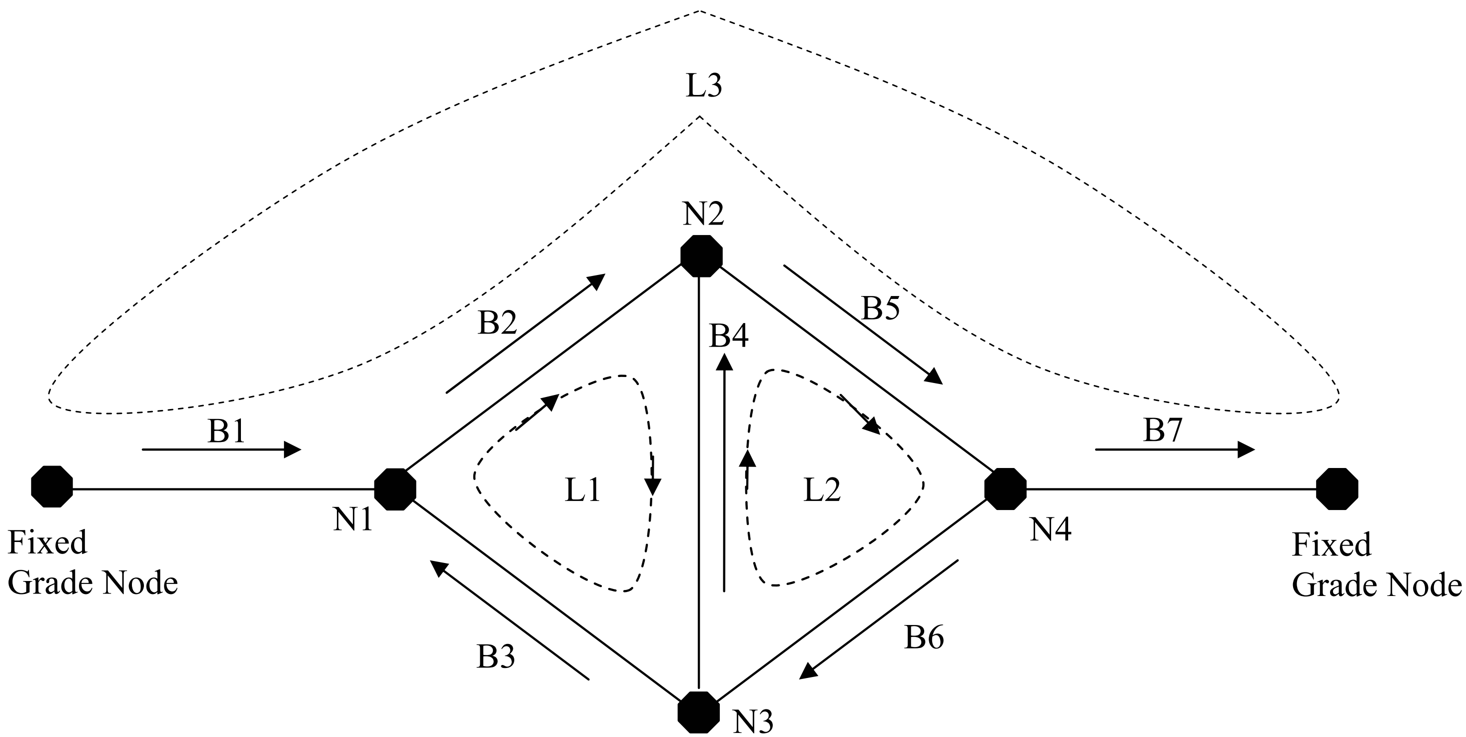
- The single path flowrate adjustment method was invented by Hardy Cross (1936).
- The network solution technique was originally used in the calculation of pipe flows.
- Steady-state or transient fluid flows in complex geometries
- Simplest mathematical structure and smallest computational effort

Novel Applications for FNM

- Hybridization with available CFD codes (*e.g.*, SPH)
- Automated design process
- Extension beyond simple pipe networks
- Use of experimental data
- Use in virtual reality demonstrations

FNM Fundamentals (I)

- Construction of a graphical network using three key elements [nodes(Ni), branches(Bi), and loops(Li)]
- Unknown variables
  - -Flow distribution in the branches
  - -Pressures at the nodes



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FNM Fundamentals (II)

Mass Conservation

$$\sum_{in} \dot{m}_i = \sum_{out} \dot{m}_i \quad \text{or} \quad \sum_{i=1}^{N+L} S_{ji}\dot{m}_i = 0 \ \ (j = 1, 2, \cdots, N)$$

$\dot{m}_i$: Mass flowrate of i^{th} branch

S_{ji} : Flow direction in i^{th} branch relative to j^{th} node

- $+1$ when fluid flows into j^{th} node
- -1 when fluid flows out of j^{th} node
- 0 when i^{th} branch has no connection with j^{th} node

N : Total number of nodes

L : Total number of loops

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FNM Fundamentals (III)

Energy Conservation

$$H_j - \sum E_p = \Delta E_j$$

H_j : Energy loss in j^{th} loop

$$H_j = \sum_{i^{th} \text{ branch in } j^{th} \text{ loop}} k_i (\dot{m}_i)^{n_i}$$

k_i : Coefficient for different head

n_i : Exponent for different head losses

E_p : Energy input in the fluids by a pump or compressor

ΔE_j : Difference in pressure head at the source nodes

No Energy Input and Head Change

$$\sum_{i=1}^{N+L} \theta_{ji} \Delta p_i = \sum_{i=1}^{N+L} \theta_{ji} K_i \dot{m}_i = 0 \quad (j = N+1,\ N+2,\ \cdots,\ N+L)$$

θ_{ji} : Similar sign convention as S_{ji}

Δp_i : Pressure drop of i^{th} branch in j^{th} loop

K_i : Globally linearized flow coefficients

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FNM Fundamentals (IV)

Globally Linearized Loop Equations

Linear equations for mass conservation
Nonlinear constitutive equations for pressure

$$\sum_i \begin{pmatrix} S_{ji} \\ \theta_{ji} K_i \end{pmatrix} \dot{m}_i = 0$$

Iterative Procedure

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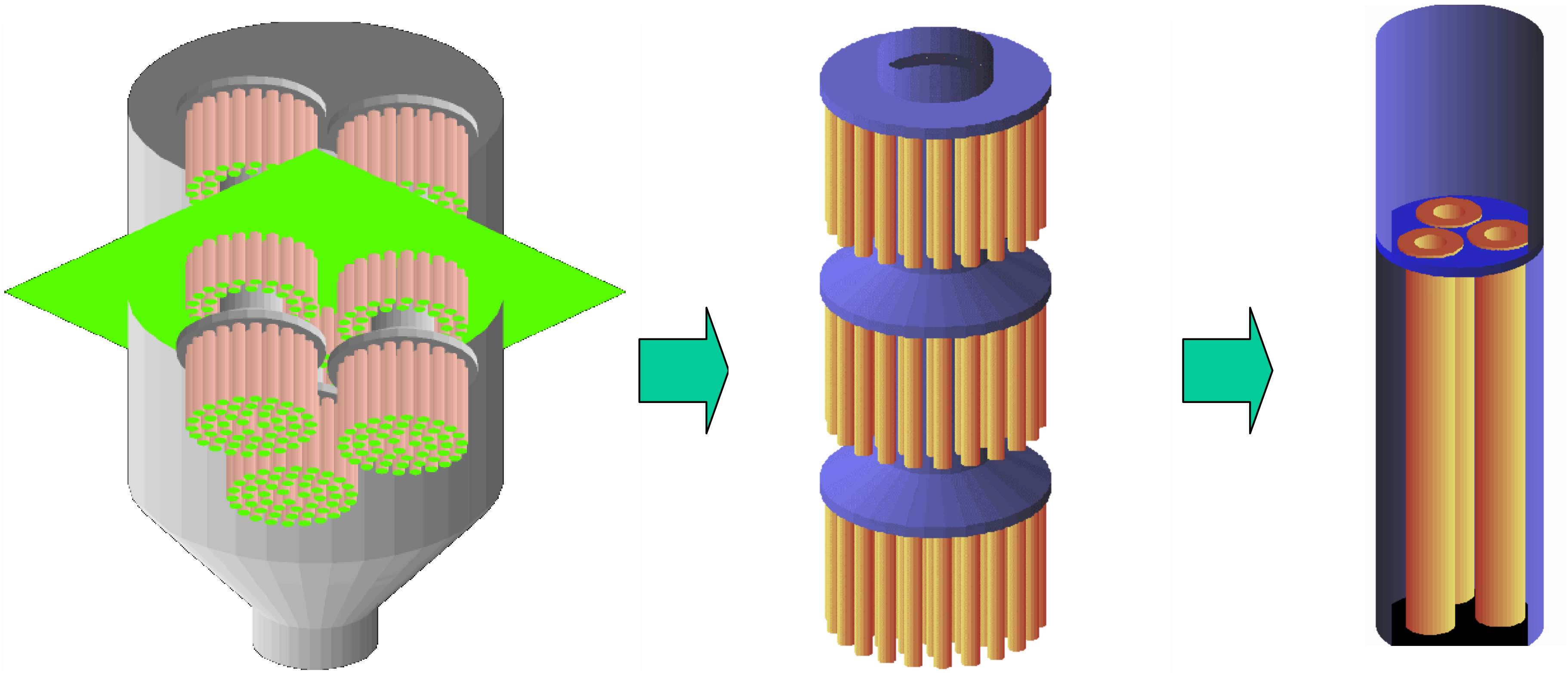
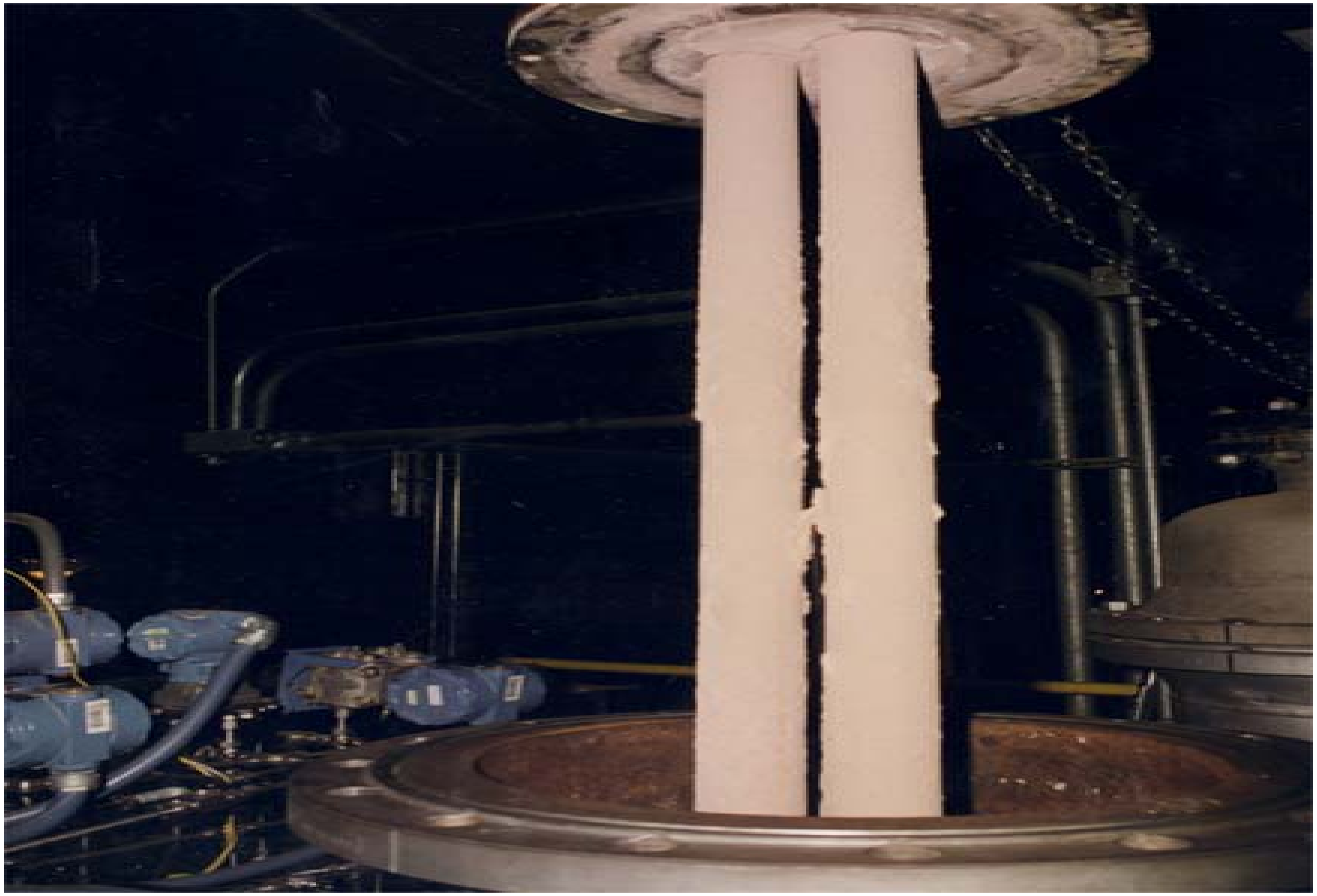
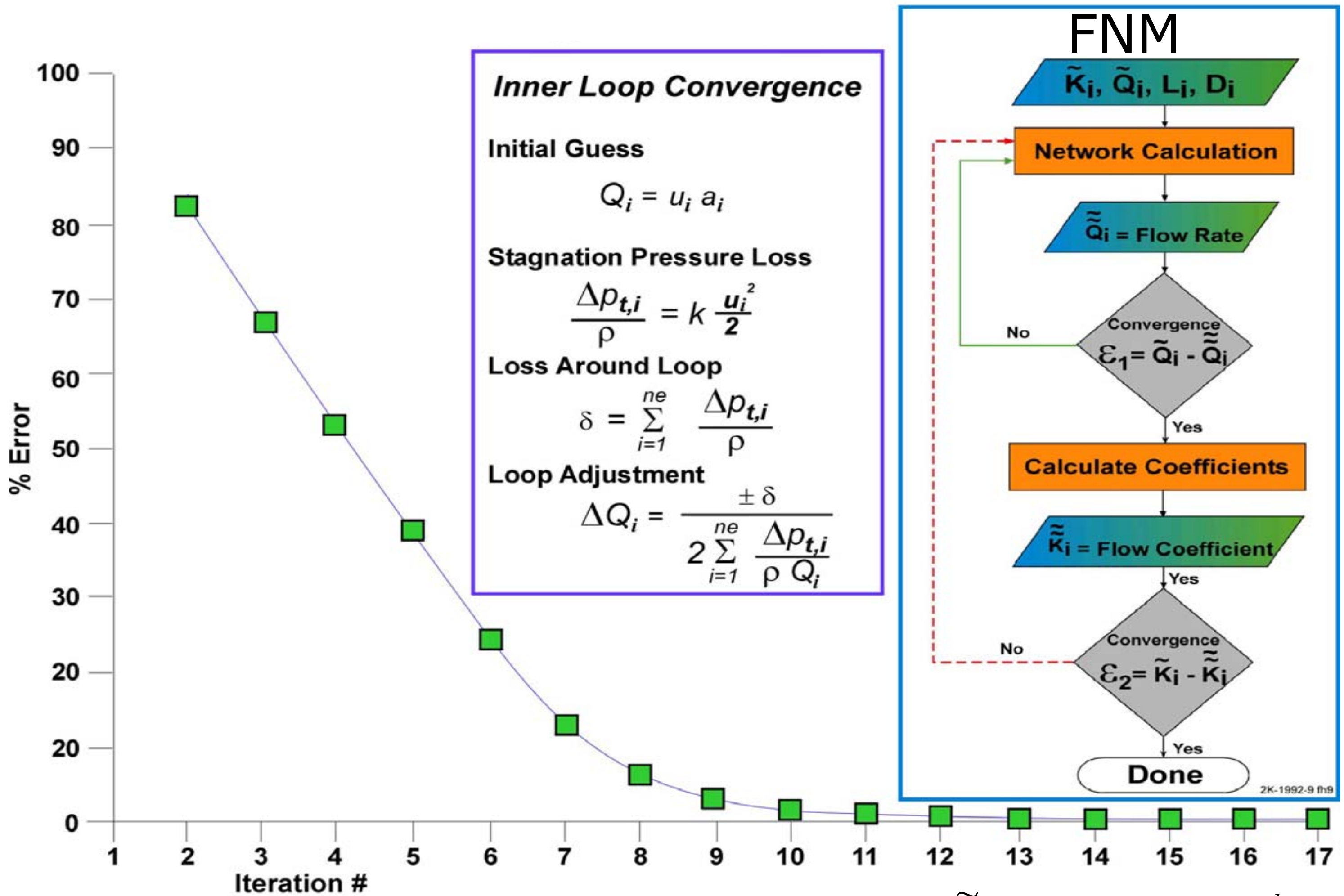
Case Study (I):
Hot Gas Filtration Unit



Filter Test Facility at NETL



FNM Convergence



Inner Loop Convergence

Initial Guess

$$Q_i = u_i \, a_i$$

Stagnation Pressure Loss

$$\frac{\Delta p_{t,i}}{\rho} = k \frac{u_i^2}{2}$$

Loss Around Loop

$$\delta = \sum_{i=1}^{ne} \frac{\Delta p_{t,i}}{\rho}$$

Loop Adjustment

$$\Delta Q_i = \frac{\pm \delta}{2 \sum_{i=1}^{ne} \frac{\Delta p_{t,i}}{\rho \, Q_i}}$$

$\tilde{A}$: Value of A at n^{th} iteration

$\tilde{\tilde{A}}$: Value of A at $(n+1)^{th}$ iteration

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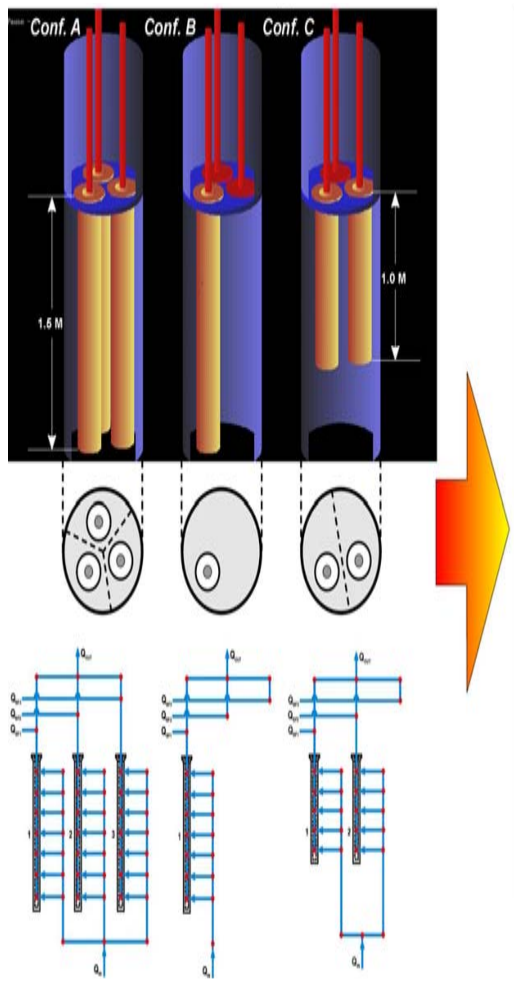
Illustration of Automated Design Process

CAD Designs | Length Scale



	Conf. A	Conf. B	Conf. C
Nfilt	3	1	2
Nsec	6	6	4
Nmed	7	7	5
Vessel Dimensions			
Lves (ft)	4.9180	4.9180	3.2787
Dves (ft)	0.6667	0.6667	0.6667
Aves (ft)	0.3491	0.3491	0.3491
Cves (ft)	2.0944	2.0944	2.0944
Lsec (ft)	0.8197	0.8197	0.8197
Lmed (ft)	0.7026	0.7026	0.6557
Filter Exterior Dimensions - (Cross-Section)			
DODfilt (ft)	0.1969	0.1969	0.1969
AODfilt (ft)	0.0304	0.0304	0.0304
COD (ft)	0.6184	0.6184	0.6184
Filter Interior Dimensions - (Cross-Section)			
DIDfilt (ft)	0.1312	0.1312	0.1312
AIDfilt (ft)	0.0135	0.0135	0.0135
CIDfilt (ft)	0.4123	0.4123	0.4123
Annulus Dimensions - (Cross-Section)			
Ablock (ft)	0.0913	0.0304	0.0609
Aopen (ft)	0.2578	0.3186	0.2882
Pwet (ft)	3.9497	2.7128	3.3312
Dhyd (ft)	0.2610	0.4698	0.3461
Annulus Section			
DsecEF (ft)	0.2610	0.4698	0.3461
AsecEF (ft)	0.0859	0.3186	0.1441
Psec (ft)	1.3166	2.7128	1.6656
Medium Section			
Aeff (ft)	0.4345	0.4345	0.4055
Leff (ft)	0.0656	0.0656	0.0656
Peff (ft)	2.6420	2.6420	2.5483
Deff (ft)	0.6578	0.6578	0.6365
Total Aspect Ratio			
AF (ft)	3.0414	3.0414	2.0276
AFtot (ft)	9.1243	3.0414	4.0552
AR tot	35.3979	9.5453	14.0710
Annulus Aspect Ratio			
ARsec	5.0568	1.3636	2.8142

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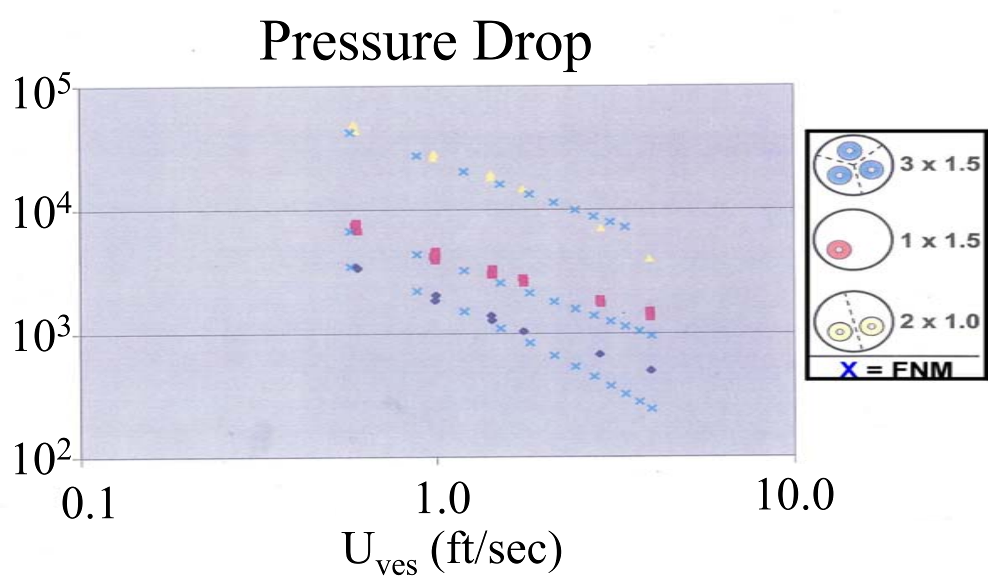
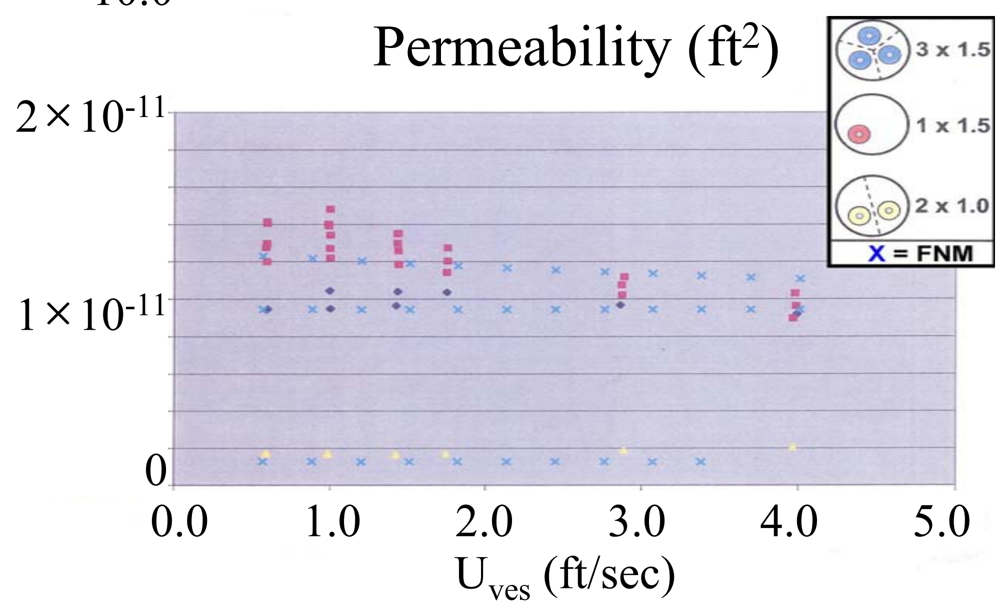
Comparison with Experiment





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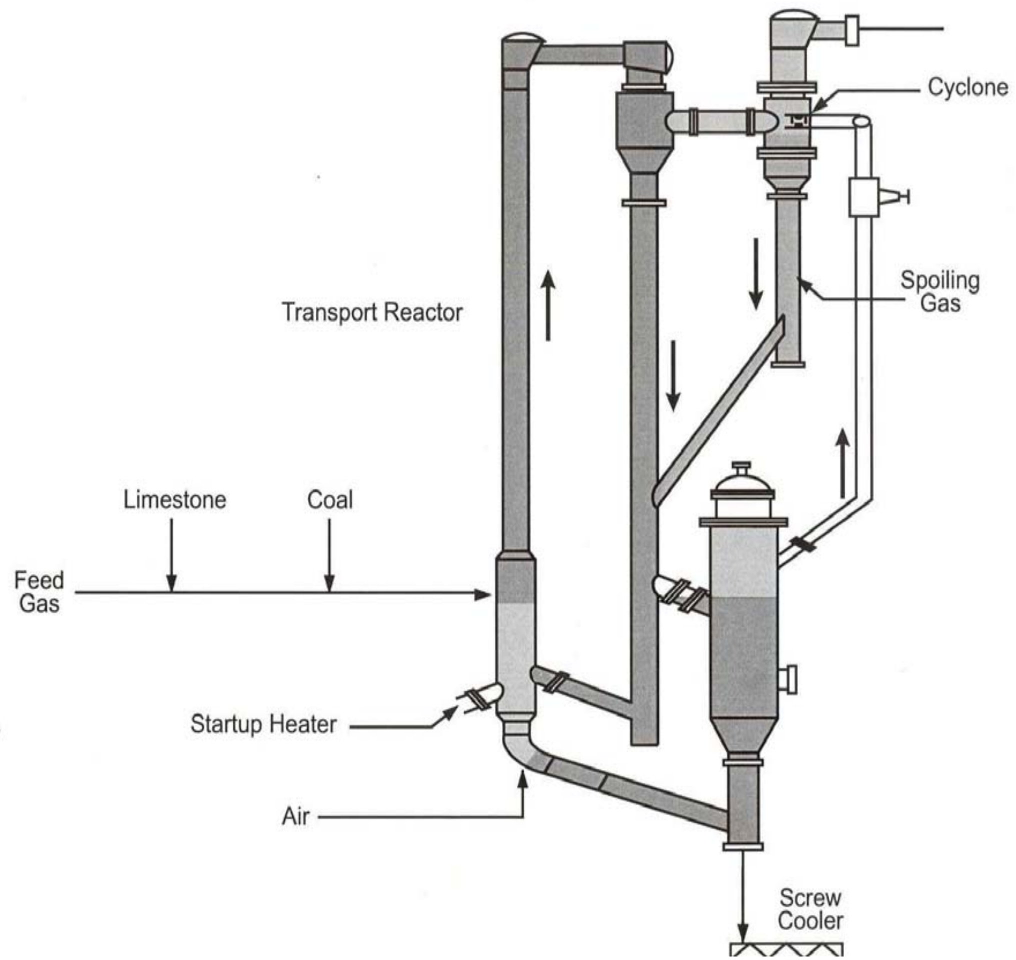
Case Study (II): Circulating Fluidized Bed System at NETL



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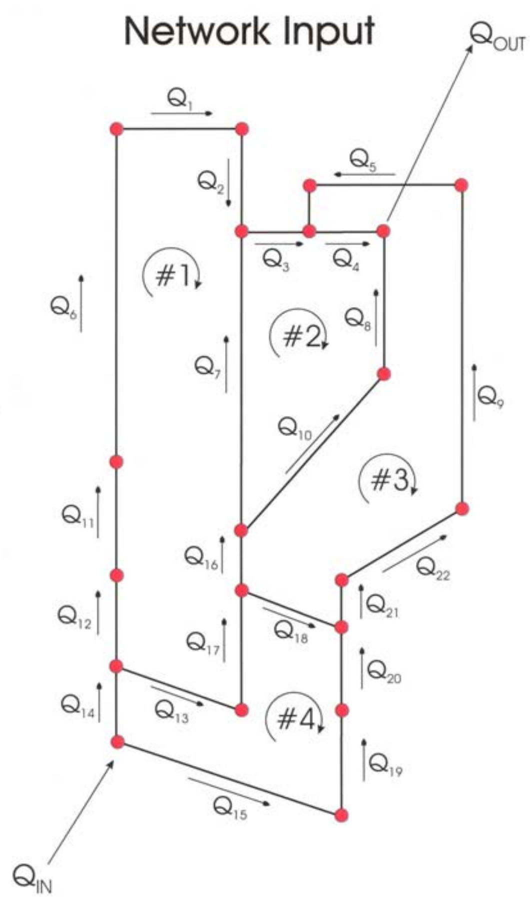
FNM Network



$$\dot{m} = \rho Q$$

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Results

Element	Length	Diameter	$\dot{m}$ (Input)	$\dot{m}$ (Output)
1	8.00	9	0.250	0.253
2	4.00	9	0.250	0.253
3	3.00	9	0.313	0.767
4	3.00	9	0.938	0.798
5	4.00	4	0.625	0.031
6	56.00	9	0.250	0.253
7	20.00	14	0.063	0.514
8	10.00	14	0.063	0.202
9	40.00	4	0.625	0.031
10	11.66	6	0.063	0.202
11	11.50	14	0.250	0.253
12	11.50	14	0.250	0.253
13	10.00	10	0.250	0.598
14	5.00	14	0.500	0.851
15	12.00	6	0.500	0.149
16	15.00	14	0.125	0.716
17	39.00	14	0.250	0.598
18	12.00	6	0.125	-0.118
19	10.00	14	0.500	0.149
20	20.00	14	0.500	0.149
21	10.00	14	0.625	0.031
22	12.00	4	0.625	0.031

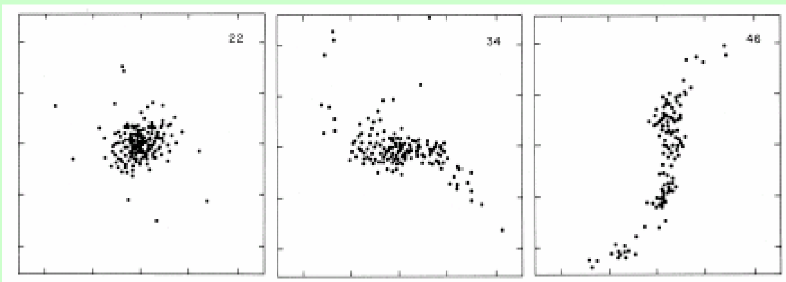
SPH Fundamentals (I)

- Breakthrough Nature
  - Lagrangian, Mesh-less, and Transient
- Easy Implementations
  - Parallelization
  - Complex geometry
  - Fluid-structure interaction
  - Turbulent & reactive fluid
- Particle/Field Hybridization
  - SPH⟺Pressure Implicit Vorticity Model on other CFD codes

SPH Fundamentals (II)

Applications of SPH

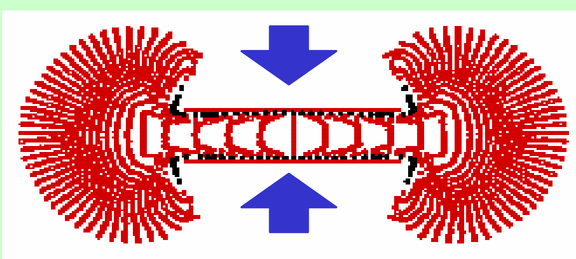
Astrophysics



Evolution of a Rotating Protostar

L. B. Lucy, "A Numerical Approach to Testing of the Fission Hypothesis," *Astron. J.* **82**, 1013, 1977.

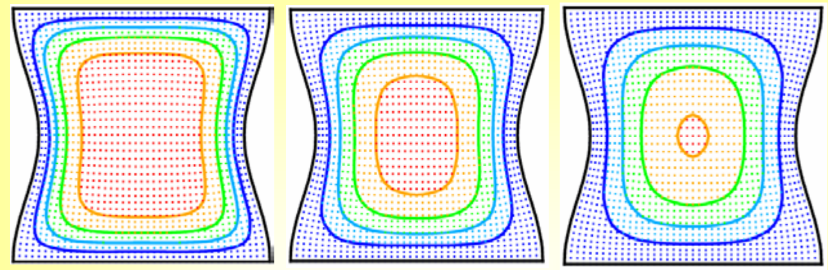
Solid Mechanics



Compression of a Hyperelastic Material

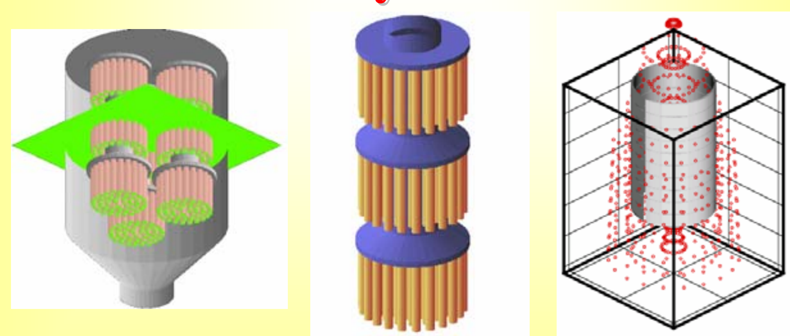
S. Li and W. K. Liu, "Meshfree and Particle Methods and Their Applications", *App. Mech. Rev.* **55**, 1, 2002.

Heat Conduction



J.H. Jeong, M.S. Jhon, J.S. Halow, and J. VanOsdol, "Smoothed Particle Hydrodynamics: Applications to Heat Conduction," *Computer Physics Communications* **153**(1), 71, 2003.

Virtual Reality Demonstration



Current Poster Presentation

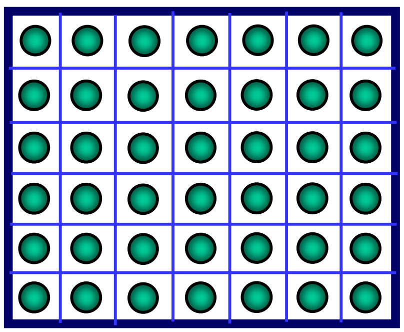
SPH Fundamentals (III)

Particle and Field Descriptions

Modeling of Multiscale Systems

Particle Dynamics

Ordinary differential equation (ODE)

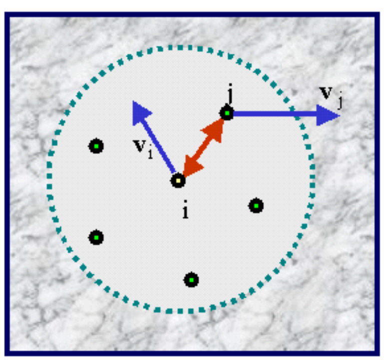


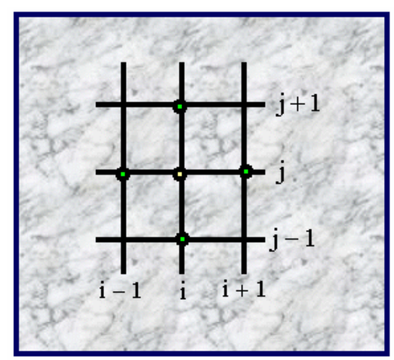
- Nanotechnology
- Particle/fluid coupling
- Chemical reaction

Field Equations

Partial differential equation (PDE)

SPH ←— **Hybrid?** —→ **CFD**





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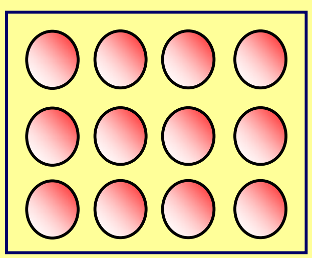
SPH Fundamentals (IV)

Fundamental Governing Equations

Particle (SPH Framework)	Field (CFD Framework)
Non-Newtonian Fluids	Non-Newtonian Fluids
$\frac{d\rho_i}{dt} = \sum m_j (\mathbf{v}_i - \mathbf{v}_j) \bullet (\nabla W)_{ij}$	$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho\, \mathbf{v}) = 0$
$\rho_i \frac{d\mathbf{v}_i}{dt} = -\sum \frac{m_j}{\rho_j}(p_i + p_j)(\nabla W)_{ij} + \sum \frac{m_j}{\rho_j}(\boldsymbol{\tau}_i + \boldsymbol{\tau}_j) \bullet (\nabla W)_{ij}$	$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \bullet \nabla \mathbf{v}\right) = -\nabla p + \nabla \bullet \boldsymbol{\tau}$
Constitutive Relationship for Newtonian Fluids	Constitutive Relationship for Newtonian Fluids
$\boldsymbol{\tau}_i = \sum \frac{m_j}{\rho_j}\left(\mu\left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T\right] + \left(\kappa - \frac{2}{3}\mu\right)(\nabla \bullet \mathbf{v})\mathbf{I}\right)_j W_{ij}$	$\boldsymbol{\tau} = \mu\left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T\right] + \left(\kappa - \frac{2}{3}\mu\right)(\nabla \bullet \mathbf{v})\mathbf{I}$
T : transpose, $\mathbf{I}$: unit dyad	T : transpose, $\mathbf{I}$: unit dyad
Incompressible Newtonian Fluids	Incompressible Newtonian Fluids
$\sum m_j (\mathbf{v}_i - \mathbf{v}_j) \bullet (\nabla W)_{ij} = 0$ or $\sum \frac{m_j}{\rho_j}(\nabla^2 p + \rho \nabla \mathbf{v} : \nabla \mathbf{v})_j W_{ij} = 0$	$\nabla \bullet \mathbf{v} = 0$ or $\nabla^2 p = -\rho \nabla \mathbf{v} : \nabla \mathbf{v}$
	

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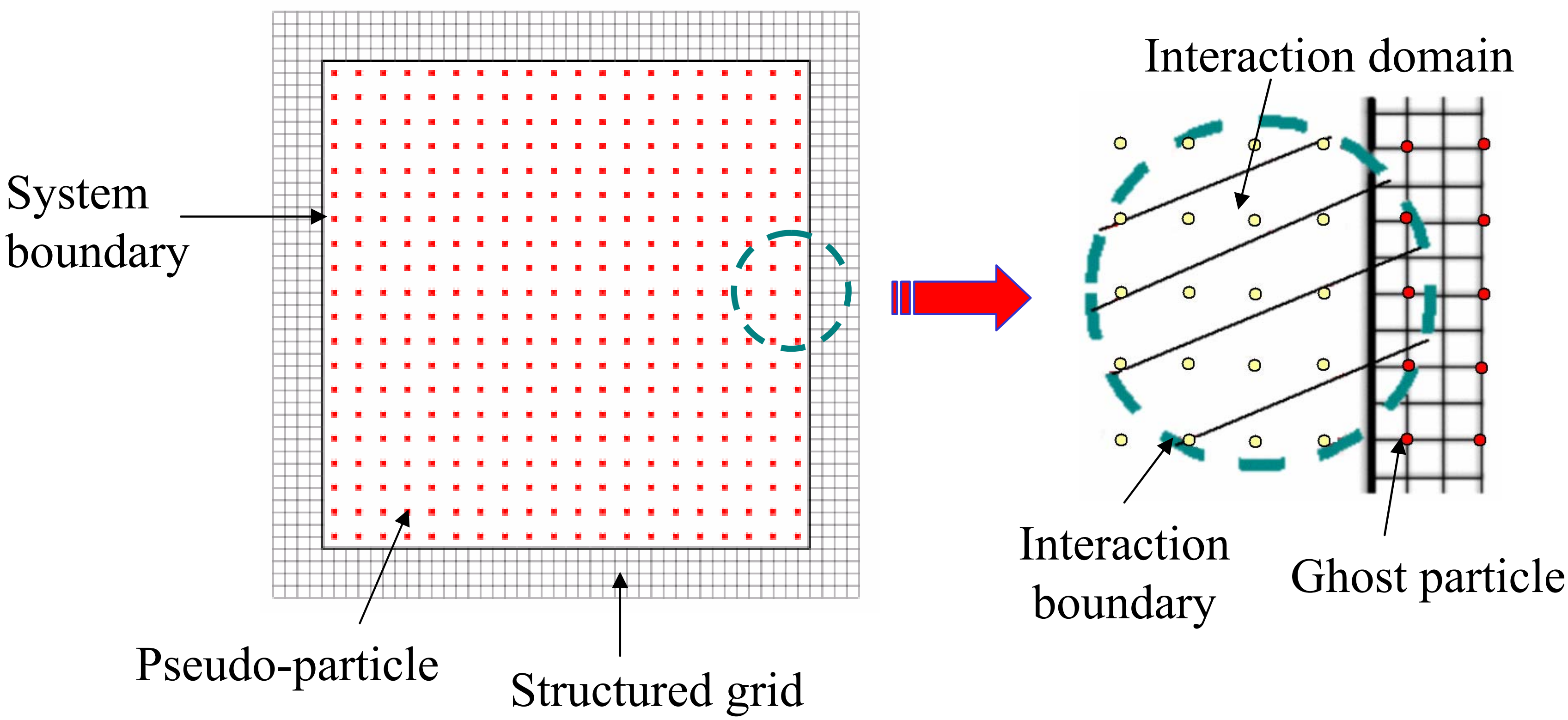
SPH Fundamentals (V)

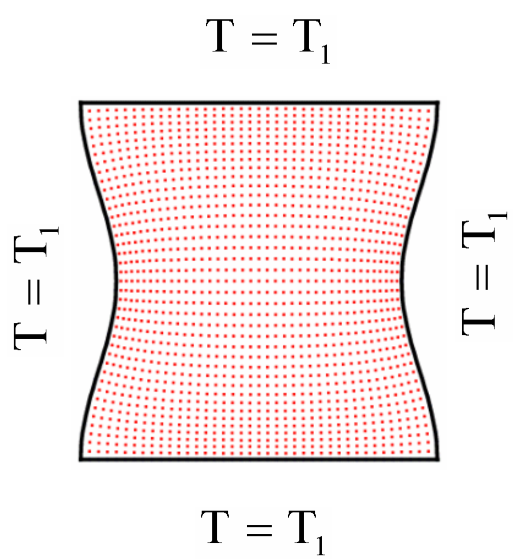
Implementation of boundary conditions:
Ghost particle method



Application: Heat Transfer

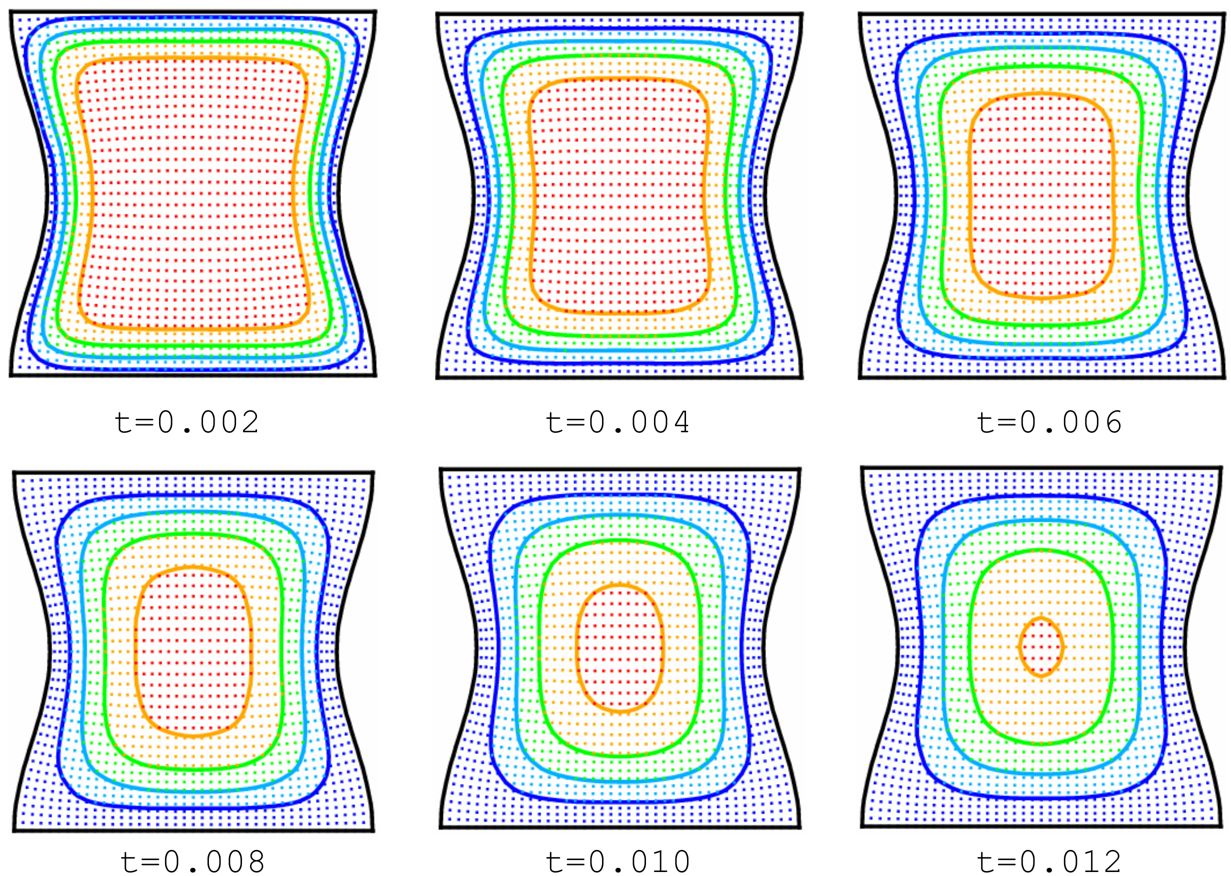
Irregular System Geometry with Dirichlet Boundary Condition

Illustration of the mesh-less nature of SPH



$$\frac{DT}{Dt} = \nabla^2 T$$

$$T = T_0 \neq T_1 \quad \text{at } t = 0$$



J.H. Jeong, M.S. Jhon, J.S. Halow, and J. VanOsdol, "Smoothed Particle Hydrodynamics: Applications to Heat Conduction," *Computer Physics Communications,* **153**(1), 71, 2003.

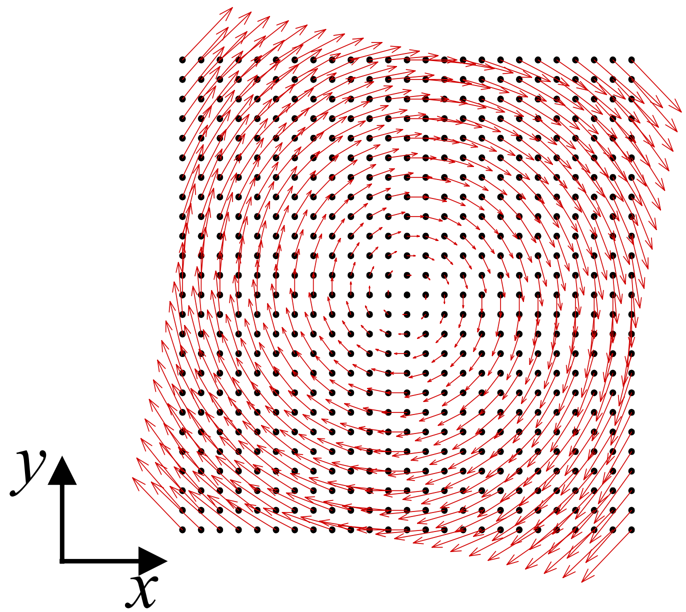
SPH Formulation in Weakly Compressible Fluids

- Mass & Momenta Balances
- Artificial Equation of State

$$P = \frac{c^2 \rho_0}{\Gamma}\left(\left(\frac{\rho}{\rho_0}\right)^{\Gamma} - 1\right)$$

P : Pressure, c : sound speed, and ρ_0 : reference density

Test Example:
2D Vortex Spin-down Flow



Reynolds number $(Re) = 420$ and $\Gamma = 7.0$

Velocity field at $t = 0$

$$\mathbf{v}(t=0) = 0.25[(y-0.5)\hat{\mathbf{i}} + (0.5-x)\hat{\mathbf{j}}]$$

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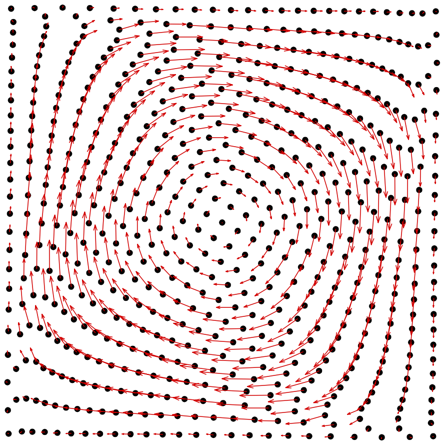
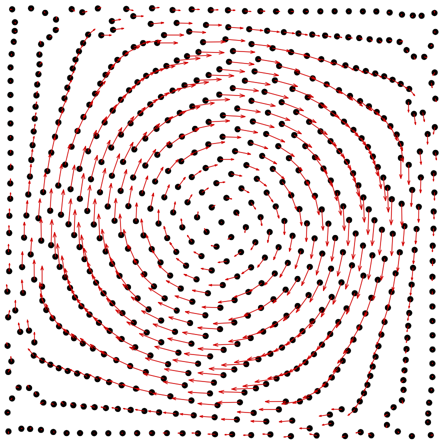
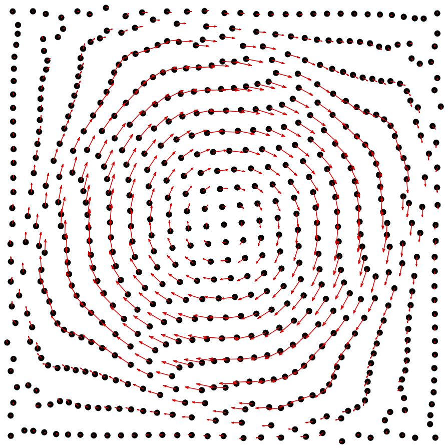
2D Vortex Spin-down Flow



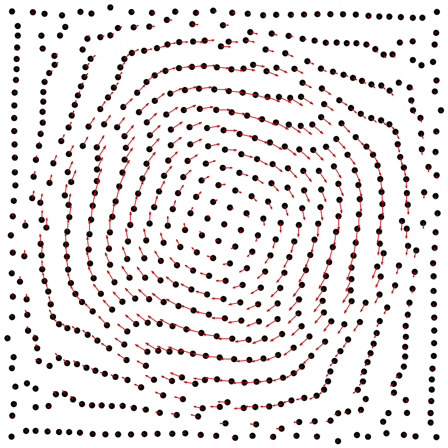
t = 2.0



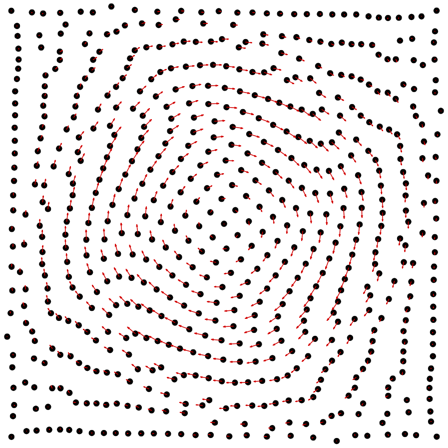
t = 4.0



t = 6.0



t = 8.0



t = 10.0

SPH Formulation with Vorticity-Stream Function Method (I)

4 Equations ⟺ 4 Unknowns ($\mathbf{v}$ and p)

or

7 Equations ⟺ 7 Unknowns ($\mathbf{v}, \boldsymbol{\omega}$, and p)

Pressure explicit (4 equations)

$$\nabla \bullet \mathbf{v} = 0,$$

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \bullet \nabla \mathbf{v}\right) = -\nabla p + \mu \nabla^2 \mathbf{v}$$

$$\boldsymbol{\omega} = \nabla \times \mathbf{v}$$

$$\mathbf{v} = \nabla \times \mathbf{A}$$

Pressure implicit (6 equations)

$$\nabla^2 \mathbf{A} = -\boldsymbol{\omega},$$

$$\rho\left(\frac{\partial \boldsymbol{\omega}}{\partial t} + \nabla \times (\boldsymbol{\omega} \times \nabla \times \mathbf{A})\right) = \mu \nabla^2 \boldsymbol{\omega}$$

3 more equations to solve for $\boldsymbol{\omega}$

1 more equation to solve for p

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Vorticity-Stream Function Formulation Using SPH

- Vorticity($\boldsymbol{\omega}$) Transport Equation
- Poisson Equation for Vector Potential (or Stream Function), **A**
- Pressure is obtained from the calculated vorticity and stream function.
- The illustration below is based on the Eulerian view.

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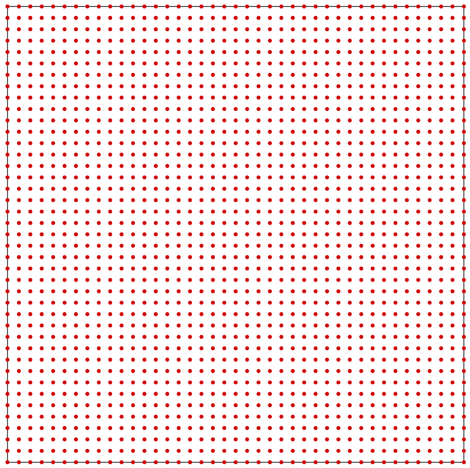
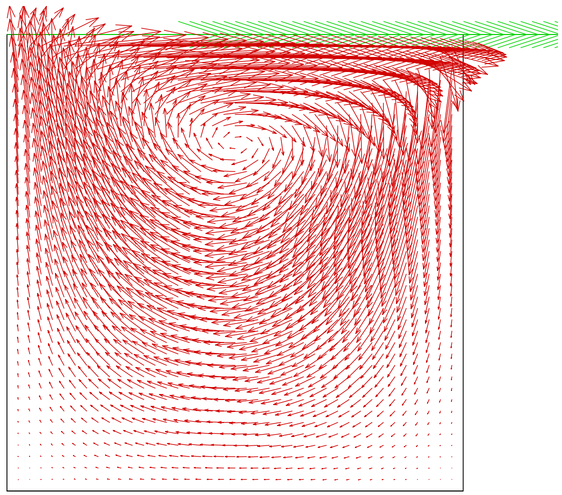
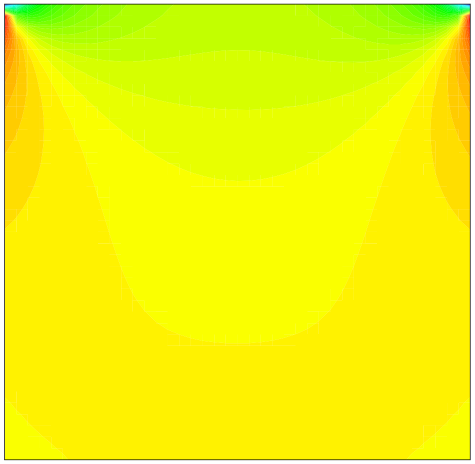
Case Study: 2D DIRF System



Pseudo-Particles

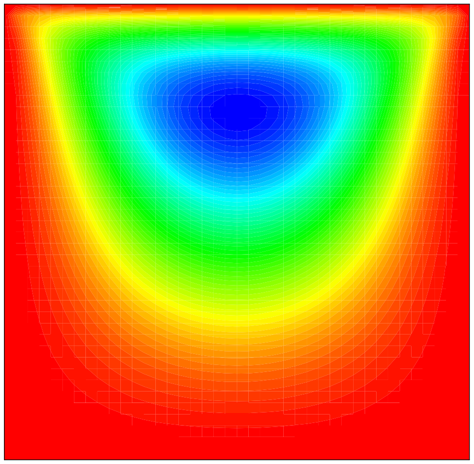


Velocity



Vorticity

$$\boldsymbol{\omega} = \omega \hat{\mathbf{k}}$$



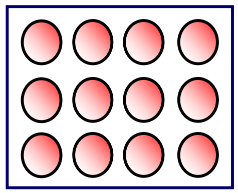
Stream Function

$$\mathbf{A} = \psi \hat{\mathbf{k}}$$

Hybridization Philosophy

Velocity

Particle Methods

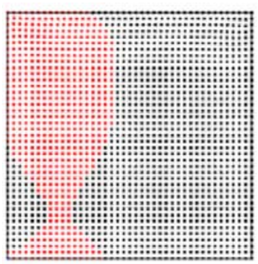


- Lagrangian
- ODEs

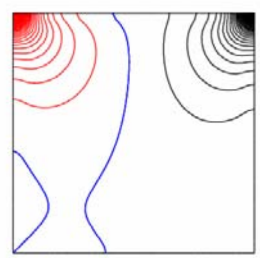
Continuum Methods

- Eulerian
- PDEs

Pressure



mapping



Particle view

Field view

An accurate estimate of pressure is a prerequisite for hybrid SPH code development.

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Particle/Field Hybridization (I)

Flow Chart

Generate the pseudo-particles.

Compute the number density of the particles.

$$n_i = \sum_j W(\mathbf{x}_j - \mathbf{x}_i) \equiv \sum_j W_{ij}$$

Solve the momenta balance equations.

$$\boldsymbol{\tau}_i = -\mu \sum \frac{1}{n_j}\left[(\nabla W)_{ij}(\mathbf{v}_i + \mathbf{v}_j) + (\mathbf{v}_i + \mathbf{v}_j)(\nabla W)_{ij}\right]$$

$$\rho_i \frac{d\mathbf{v}_i}{dt} = \sum \frac{1}{n_j}(p_i + p_j)(\nabla W)_{ij} - \sum \frac{1}{n_j}(\boldsymbol{\tau}_i + \boldsymbol{\tau}_j)\bullet(\nabla W)_{ij} + \sum \frac{1}{n_j}\mathbf{F}_j^g W_{ij}$$

Pressure input

obtain p from mapping

PIVM or FNM

Update the positions of the particles.

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \text{ or } \mathbf{x}_i = \int \mathbf{v}_i dt$$

$\mathbf{x}_i$ and $\mathbf{v}_i$

PIVM: Pressure Implicit Vorticity Method

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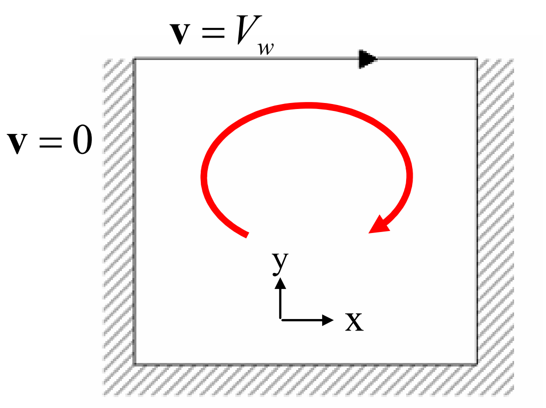
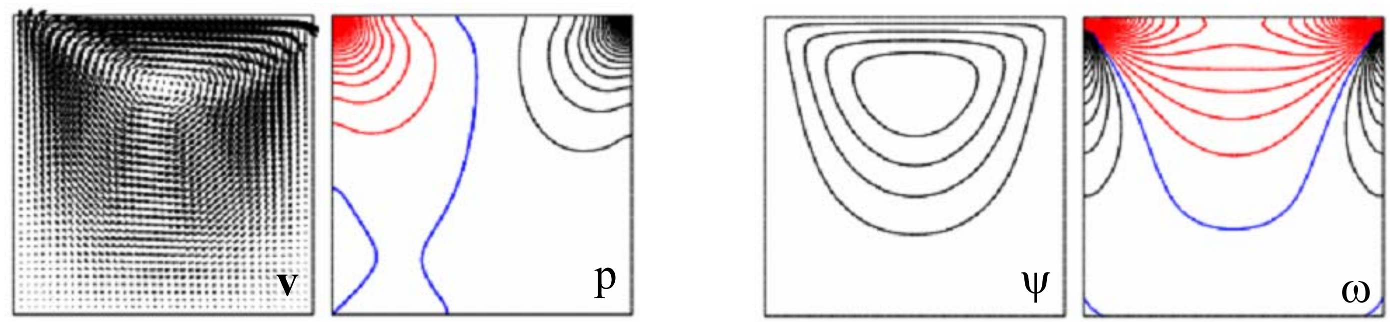
Particle/Field Hybridization (II)

2D Test Example



$Re = 1$

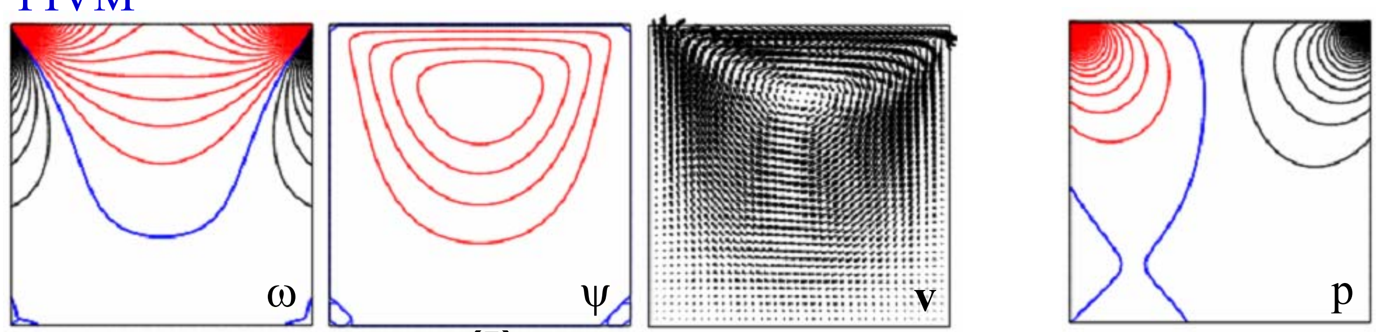
FLUENT



(I) (II)

FNM???

PIVM



(I) (II)

$$\rho \frac{D\omega}{Dt} = \mu \nabla^2 \omega$$

$$\mathbf{v} = \nabla \times (\psi \ \mathbf{e}_3)$$

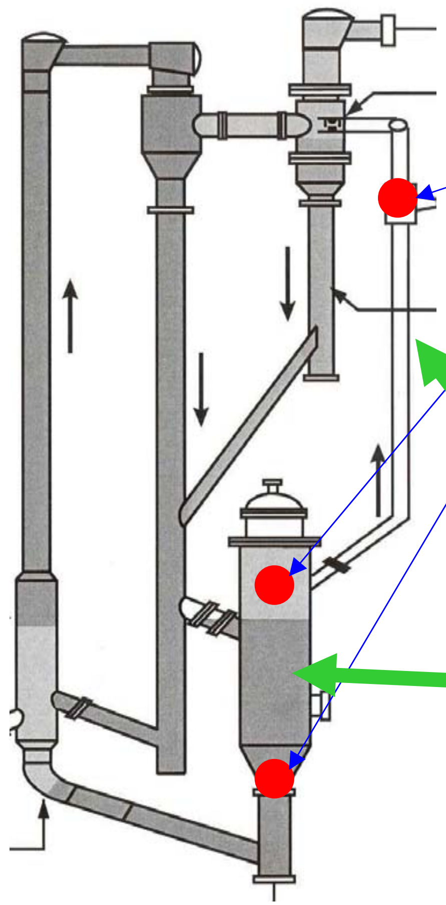
$$\nabla^2 \psi = -\omega$$

$$\nabla^2 p = -\rho \nabla \mathbf{v} : \nabla \mathbf{v}$$

- FLUENT and PIVM results complement one another with nearly identical convergence times.
- When a velocity boundary condition is imposed, PIVM may be superior.
- How about SPH/FNM hybridization?

Particle/Field Hybridization (III)

Top to Bottom Approach



Pressure Calculation:
From FNM (Global Feature of the System)

Hybridization

Velocity Calculation:
From SPH (Local Flow Feature inside Each Component)

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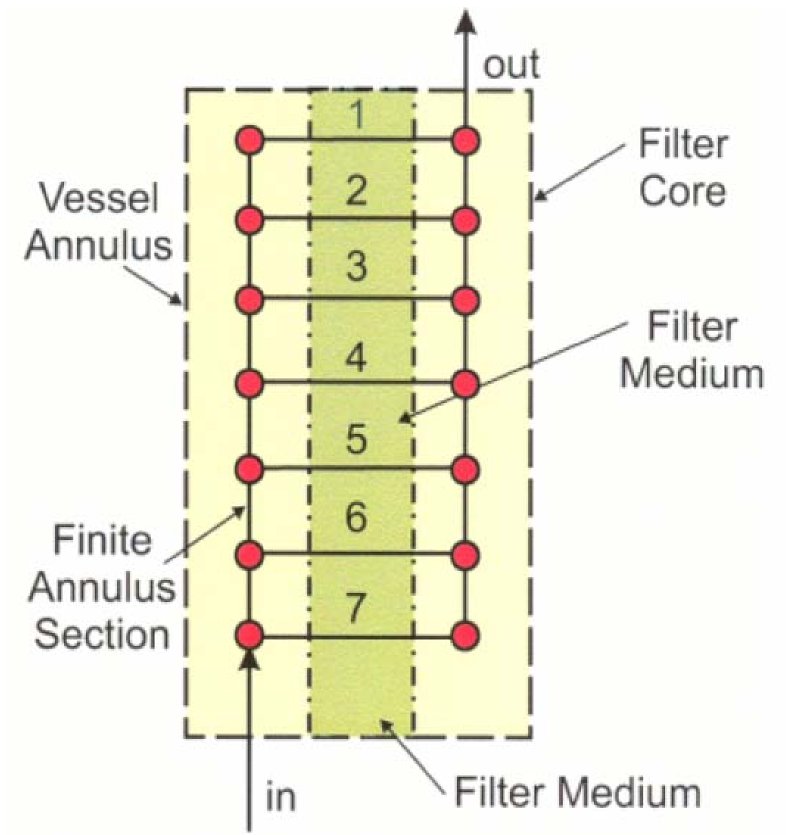
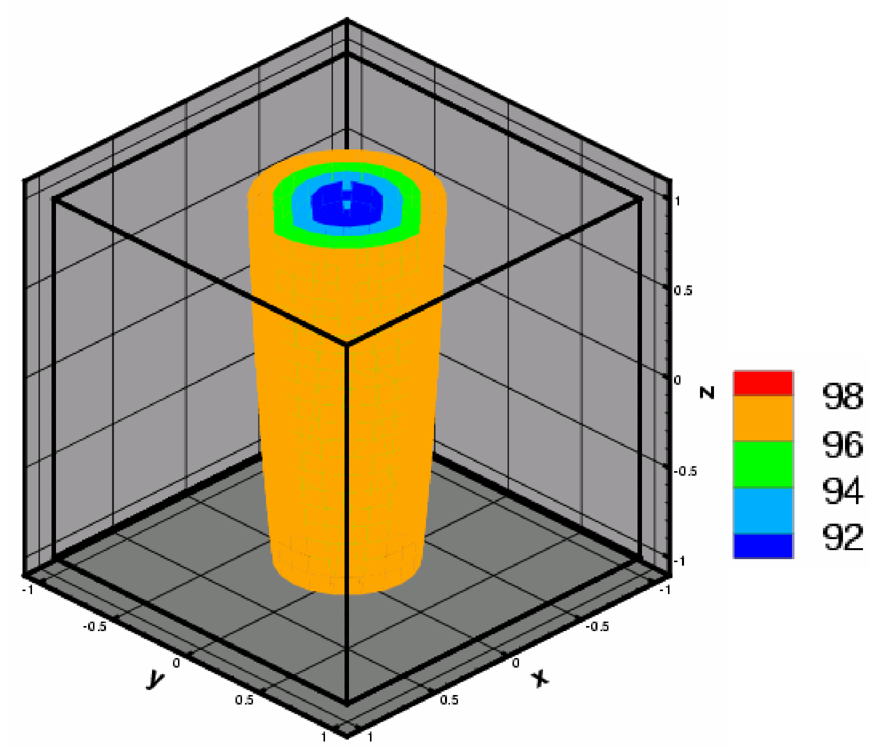
Virtual Reality Demonstration (I)





3D Pressure profile via FNM

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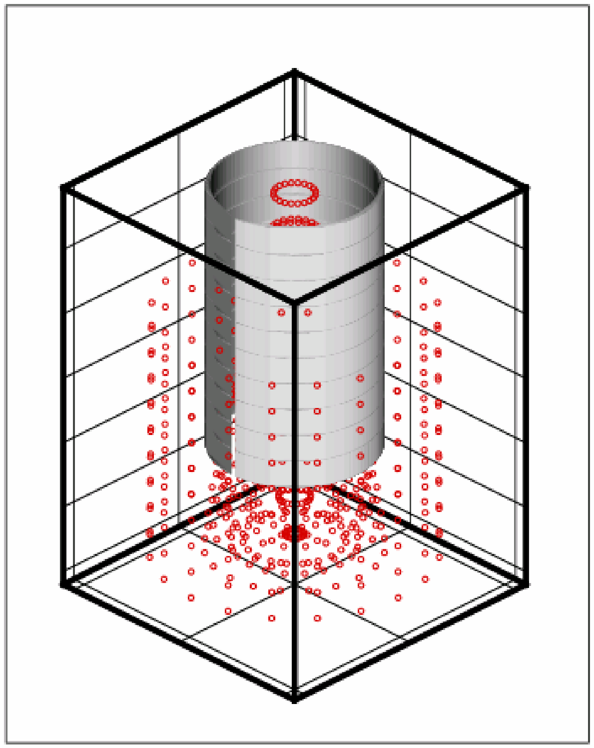
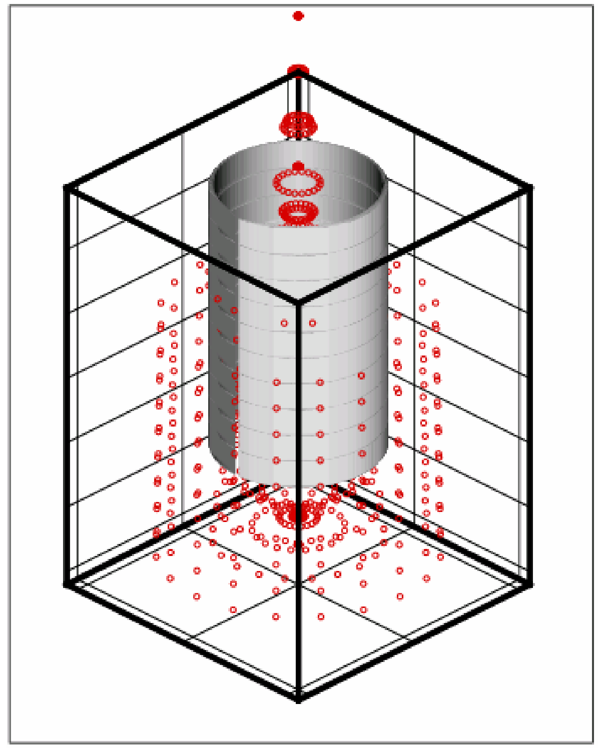
Virtual Reality Demonstration (II)





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Conclusion

- The development of a CFD code that links geometrical CAD software to an FNM/SPH for the general design process is discussed.
- A generalized FNM method suitable for hybridizing CFD codes is constructed.
- The capabilities of FNM is illustrated by two case studies; hot gas filtration & circulating fluidized bed test facilities at NETL.
- SPH fundamentals (including the weakly compressible flow and novel vorticity formulation) have been examined.
- The essence of SPH formulation is illustrated via test examples.
- FNM & SPH coupling codes suitable for virtual reality demonstrations are currently under construction.

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