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# Micro/Meso simulations of a fluidized bed with heat transfer

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# Micro/Meso simulations of a fluidized bed with heat transfer

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Fluidization XV.
2016 – Montebello, Canada

ANR MORE4LESS

# Gas-solid flows in industry

- Fields :

| Energy | Chemistry<br>Petrochemicals | Pharmaceutics<br>Food |
|---|---|---|
| Cracking | Reactors | Drying |
| AA-CAES | Regenerator | Granulation |
| Solar plant | Adsorption | Coating |

- Technologies :
  - Fluidized beds
  - Fixed beds

# Gas-solid flows in industry

| | Inlet (m) | Height (m) | $N_{particles}$ |
|---|---|---|---|
| Pilot plant[1] | $0.254 \times 0.432$ | 3 | $10^{9} - 10^{11}$ |
| Industrial plant[2] | 5 | 22 | $10^{13} - 10^{15}$ |

*PeliGRIFF* (*IFPEN*)

*YALES*2 (*CORIA*)

*NEPTUNE_CFD* (*IMFT*)

- ANR project MORE4LESS : IFPEN, CORIA, IMFT

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[1] Fournol and Bergougnou. In: *Can. J. Chem. Eng.* 51 (1973), pp. 401–404.

[2] Farrauto Bartholomew. *Fundamentals of Industrial Catalytic Processes*.

# PeliGRIFF : Mass and momentum equations

Amir Esteghamatian
$3^{rd}$ year PhD student[3]

- Microscale : Local conservation equations

$$\nabla \cdot \boldsymbol{u_c} = 0$$

$$\frac{\partial \rho_c \boldsymbol{u_c}}{\partial t} + \nabla \cdot (\rho_c \boldsymbol{u_c} \boldsymbol{u_c}) + \nabla P - \mu_c \nabla^2 \boldsymbol{u_c} - \rho_c \boldsymbol{g} + \boldsymbol{F_{loc}} = 0$$

- Mesoscale : Averaged conservation equations

$$\frac{\partial \alpha_c}{\partial t} + \nabla \cdot (\alpha_c \boldsymbol{u_c}) = 0$$

$$\frac{\partial \alpha_c \rho_c \overline{\boldsymbol{u_c}}}{\partial t} + \nabla \cdot (\alpha_c \rho_c \overline{\boldsymbol{u_c} \boldsymbol{u_c}}) + \nabla P - \nabla \cdot (\alpha_c \boldsymbol{\tau_c}) + \overline{\boldsymbol{F_{pc}}} - \alpha_c \boldsymbol{g} = 0$$

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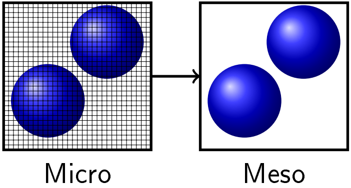
[3] Esteghamatian et al. “Micro/Meso simulation of a fluidized bed in a homogeneous bubbling regime”. In: *Int. J. Mult. Fl.* (2016).

# PeliGRIFF : Temperature equation



- Microscale : Local conservation equations

$$\frac{\partial \rho_c Cp_c T_c}{\partial t} + \nabla \cdot (\rho_c Cp_c T_c \boldsymbol{u_c}) - \nabla \cdot (\lambda_c \nabla T_c) - Q_{loc} = 0$$

- Mesoscale : Averaged conservation equations

$$\frac{\partial \alpha_c \rho_c Cp_c \overline{T_c}}{\partial t} + \nabla \cdot (\alpha_c \rho_c Cp_c \overline{T_c}\,\overline{\boldsymbol{u_c}}) - \nabla \cdot (\alpha_c \lambda_c \nabla \overline{T_c}) - \overline{Q} = 0$$

# Plan

- I- Microscale simulations
  - I-1. PeliGRIFF tools
  - I-2. Random beds
  - I-3. From DNS to DEM/CFD
- II- Comparison DNS-DEM/CFD
  - II-1. Mesoscale : Closure laws
  - II-2. Random beds
  - II-3. Fluidized beds
- Conclusion/Perspectives

# Plan

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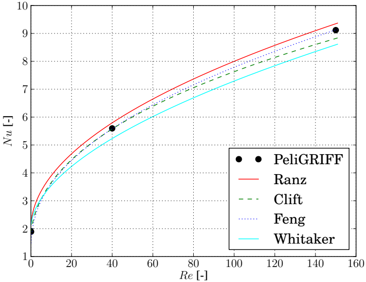
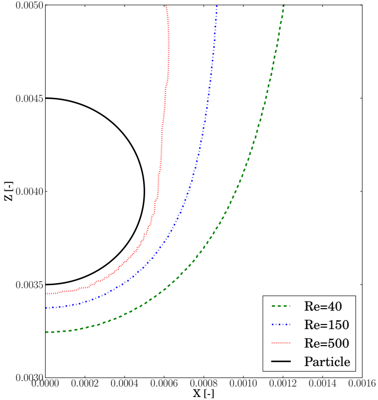
# I-1. PeliGRIFF tools : Validation (Isolated sphere)

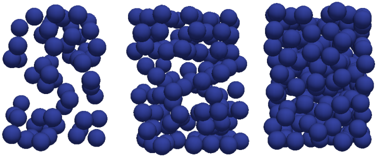
- Convergence order $p \approx 1.5$
- Error to correlations :
  - $\epsilon < 1\%$ avec Feng
  - $\epsilon \approx 3\%$ autres
- Thermal boundary layer : 4 points to get $\epsilon < 2\%$



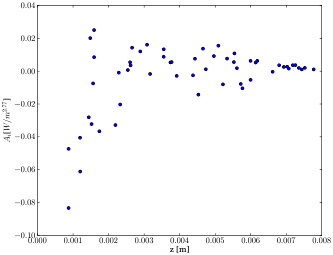


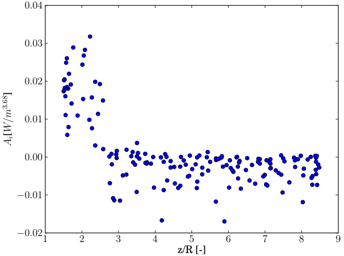
# I-2. PeliGRIFF tools : Validation (Random beds)

- Tavassoli cases[4] :
    - Bi-periodic box : $6d_p \times 6d_p \times 8d_p$
    - Grid size : $d_p/h \in [8; 64]$
    - Richardson extrapolation **$\phi_{tot}$** :
    $\phi_{tot}(h) = \phi_{tot,0} + A_{tot} h^p$



- **Individual** convergence
$\phi_i \rightarrow d_p/h = 48$ to get $\epsilon < 5\%$





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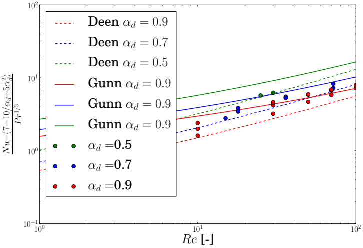
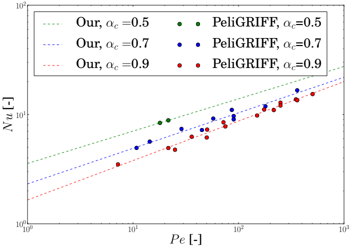
[4] Tavassoli et al. In: *Int. J. Mult. Fl.* 57 (2013), pp. 29–37.

# I-2. Random beds





- Closure laws :
  - Comparison to literature correlations : Gunn[5], Deen[6]
  - Proposition of a new closure law :

$$Nu(\alpha_d, Pe) = (1.92\alpha_d^2 + 2.27\alpha_d + 4.97)Pe^{0.42\alpha_d^2 - 0.43\alpha_d + 0.36}$$

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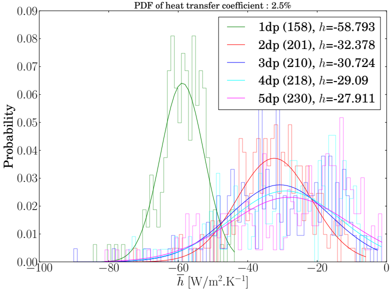
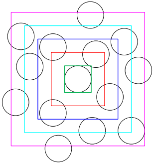
[5] Gunn. In: *Int. J. H. M. Tr.* 21 (1978), pp. 467–476.

[6] Deen and Kuipers. In: *Chem. Eng. Sc.* 116 (2014), pp. 645–656.

# I-2. Random beds





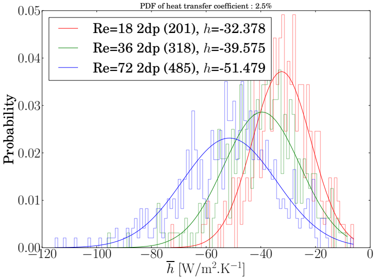
- Nusselt number definition :

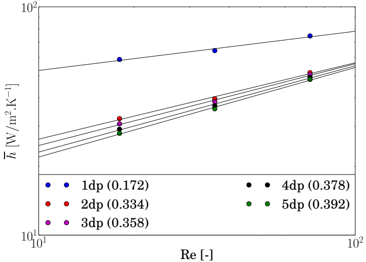
$$Nu_i = h_i S_i ( T_{d,i} - \boldsymbol{T_{c,bulk}} )$$

- Volume averaging on boxes around particles :

$$T_{c,bulk} = \frac{\int_{V_{box}} \alpha_c(\mathbf{r}) T_c(\mathbf{r}) \mathrm{d}\mathbf{r}}{\int_{V_{box}} \alpha_c(\mathbf{r}) \mathrm{d}\mathbf{r}}$$

# I-2. Random beds





- New closure law formulation $\overline{h}$ with $Re$ :

$$\overline{h} = ARe^{\alpha(L_{box}/d_p)}$$

- High impact of box size on $\alpha(L_{box}/d_p)$
- Trend with $Re$ similar to 1D-balance, Gunn[7] and Deen[8]

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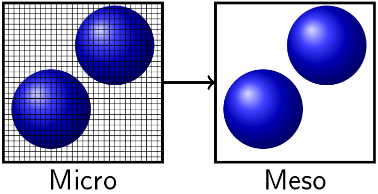
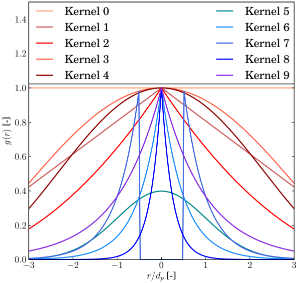
[7] Gunn. In: *Int. J. H. M. Tr.* 21 (1978), pp. 467–476.

[8] Deen and Kuipers. In: *Chem. Eng. Sc.* 116 (2014), pp. 645–656.

# I-3. From DNS to DEM-CFD





- Use of kernel weighting $g(|\boldsymbol{r}-\boldsymbol{r}_p|)$ :

$$T_{c,bulk} = \frac{\int_{V_{box}} \alpha_c(\boldsymbol{r}) g(|\boldsymbol{r}-\boldsymbol{r}_p|) T_c(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}}{\int_{V_{box}} \alpha_c(\boldsymbol{r}) g(|\boldsymbol{r}-\boldsymbol{r}_p|) \mathrm{d}\boldsymbol{r}}$$

- 10 kernel types : 5 function of box size, 5 with fixed decreasing rate
- Estimation of new closure laws depending on kernel definition

# Plan

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Conclusion/Perspectives

# II-1. Closure laws for mesoscale

- Flow : Beetstra[9], Di Felice[10], ...

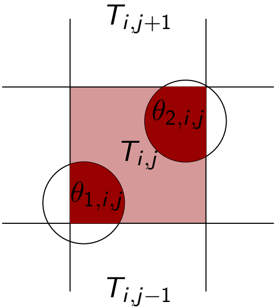
$$f_{hd} = f(\alpha_d, Re)$$

- Temperature : Gunn[11], Deen[12], ...

$$Nu_{hd} = f(\alpha_d, Re, Pr)$$

- Particle → fluid information :
  - Linear interpolation

$$Nu_{pd} = \frac{1}{\Delta V} \sum_{N_p} \theta Nu_{hd}$$



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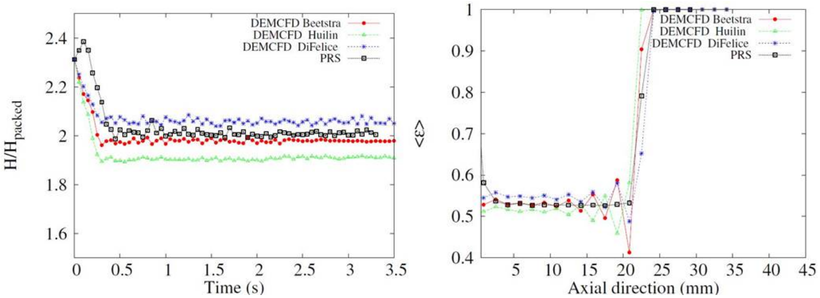
[9] Beetstra, Van der Hoef, and Kuipers. In: *Chem. Eng. Sc.* 62 (2007), pp. 246–255.

[10] Di Felice. In: *Int. J. Mult. Fl.* 20 (1994), pp. 153–159.

[11] Gunn. In: *Int. J. H. M. Tr.* 21 (1978), pp. 467–476.

[12] Deen and Kuipers. In: *Chem. Eng. Sc.* 116 (2014), pp. 645–656.

# II-2. Quid for hydrodynamic forces[14] ?



- Impact of closure laws on global parameters
- Effect of meshes to particle ratio[13]
    - Convergence for $\Delta_x / d_p \in [1.8; 3]$

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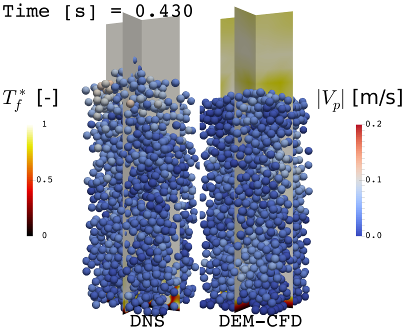
[13] Manuel Bernard. "Approche Multi-échelle pour les écoulements fluide-particules". PhD thesis. MEGEP, 2014.

[14] Esteghamatian et al. "Micro/Meso simulation of a fluidized bed in a homogeneous bubbling regime". In: *Int. J. Mult. Fl.* (2016).

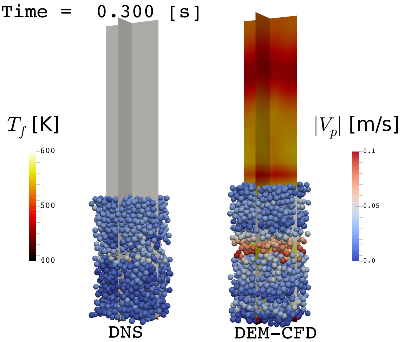
# II-2. Comparison of homogeneous fluidization



|  | DNS | DEM-CFD |
|---|---|---|
| $N_{cells}$ | $50.10^6$ | 756 |
| $N_{procs}$ | 128 | 1 |
| Time [h] | 360 | 2 |

- Heat closure law : Ranz-Marshall, Gunn
- Fluid closure law : Di Felice
- Homogeneous fluidization :
  - Particle motion and agitation : ✓
  - Heat transfer mechanisms : ≈ ✓

# II-2. Comparison of bubbling fluidization



| | DNS | DEM-CFD |
|---|---|---|
| $N_{cells}$ | $70.10^6$ | 625 |
| $N_{procs}$ | 256 | 1 |
| Time [h] | 1500 | 2 |

- Heat closure law : Ranz-Marshall, Gunn
- Fluid closure law : DiFelice
- Bubbling fluidization :
  - Particle motion and agitation : X
  - Heat transfer mechanisms : X

# Conclusion and Perspectives

- Micro-analysis of heat transfer → closure laws
- Improvement for DEM-CFD :
  - Closure laws
  - Modeling (equations)
- Direct comparison of DNS/DEM-CFD simulations on going
- Perspectives :
  - Closure laws for wall-gas heat transfer from DNS
  - Effect of bi-dispersity
- MORE4LESS Project :
  - Closure laws implementation in YALES2 (CORIA)
  - Fluidized bed with complex geometries simulations
  - DEM-CFD → Euler-Euler transition on NEPTUNE_CFD (IMFT)

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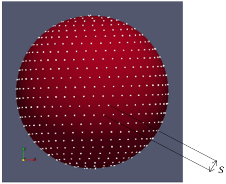
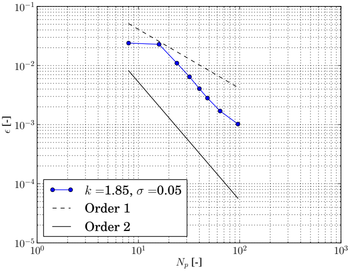
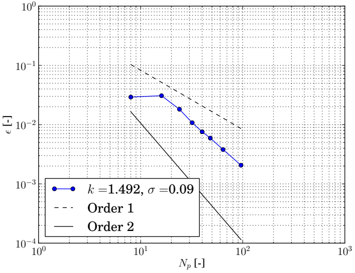
# Appendix 1. DLM/FD points distribution over a sphere

- Strategies : (layers, spiral), spacing ($s = h, 2h$)
- Spatial convergence :
  - isolated sphere, domain ($6d_p \times 6d_p \times 8d_p$)
  - Bi-perdiodic
  - Spiral distribution chosen
  - Spacing $s$ : $2h$, $\sqrt{3}h$
- Richardson : $\phi(h) = \phi_{h=0} + Bh^p$



(a) Spiral



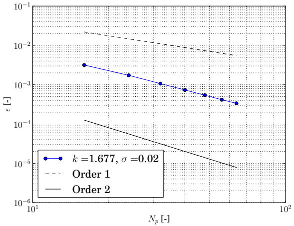


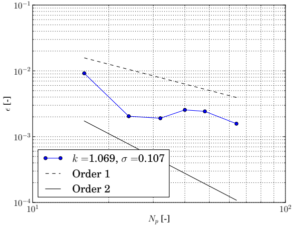
# Appendix 2 : Fixed beds spatial convergence

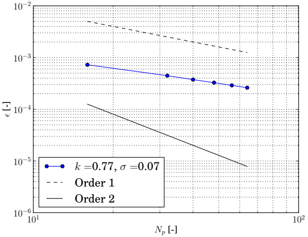
- Total heat transfer :

$$\phi_{tot} = \sum_{i=1}^{N_p} \phi_{h=0} + \sum_{i=1}^{N_p} B_i h^{p_i}$$

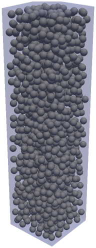
- 7 meshes (CFL constante)
- Convergence on $\phi_{tot}$



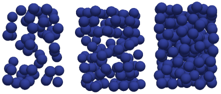




# Appendix 3 : Fixed beds heat transfer



- Deen[15] test case :
  - 1326 spheres of 6mm, $\alpha_d = 0.3$ with walls
  - $Re_s = \frac{\rho U_s d_p}{\mu_f} \in [36; 144]$
- Tavassoli[16] test case :
  - $\alpha_d \in [0.1; 0.3]$ (55 to 265 spheres of 1mm) Bi-periodic
  - $Re_s \in [10; 100]$



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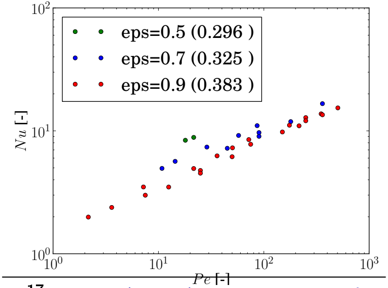
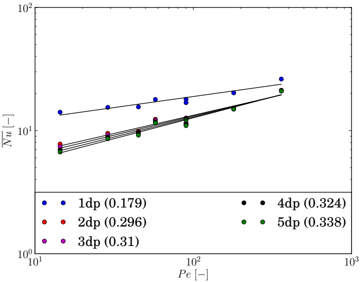
[15] Niels G. Deen et al. In: *Chem. Eng. Sc.* 81 (2012), pp. 329–344.

[16] Tavassoli et al. In: *Int. J. Mult. Fl.* 57 (2013), pp. 29–37.

# Appendix 4 : Macro/micro heat transfer analysis comparison

| Authors | Tavassoli[17] | Deen[18] |
|---|---|---|
| $\alpha_p$ | [0.1; 0.5] | 0.3 |
| $N_p$ | [55; 265] | 1326 |
| $Re_p$ | [10;100] | [36;144] |





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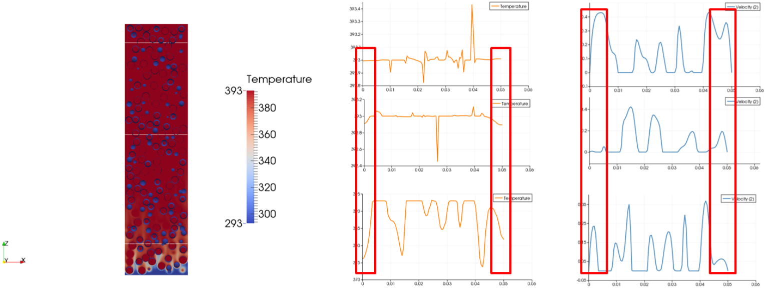
[17] Tavassoli et al. In: *Int. J. Mult. Fl.* 57 (2013), pp. 29–37.

[18] Niels G. Deen et al. In: *Chem. Eng. Sc.* 81 (2012), pp. 329–344.

# Appendix 5. Wall-Fluid heat transfer

- Literature → Glicksman[19] :
- $Nu = \frac{h_w d_p}{\lambda_c} = \begin{cases} 5 + 0.05 Re_p Pr & \text{si } \mathrm{Re_p} < 150 \\ 0.18 Re_p^{0.8} Pr^{0.33} & \text{si } \mathrm{Re_p} \geq 150 \end{cases}$



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[19] Kunii and Levenspiel. *Fluidization Engineering*. Ed. by H. Brenner. Butterworth-Heinemann, 1991.