Meso-scale Structure and Multi-scale Strategy in Simulating Multiphase Systems

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Outline of presentation

Challenges

Modeling

Meso-scale

Multi-scale
+
Discrete

Common nature

Computation

Low efficiency
High cost

Software
Hardware

Similarity in structure

Strategy

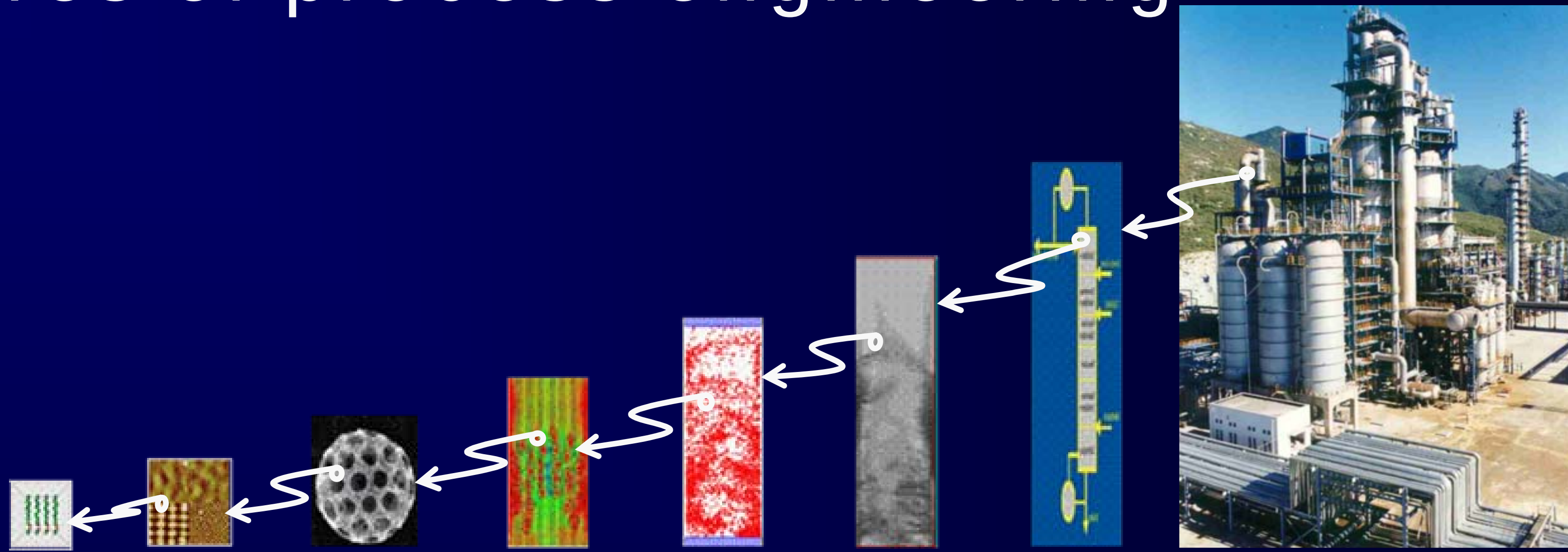
Multi-Scale
Parallel Computation

Progresses
1.0 Peta flops

Applications

Perspectives

Multi-scale and multi-level features of process engineering



Multi-scale:

Molecule ~1A | Assembly ~1 nm | Particle (~1μm) | Cell (~1mm) | Cluster (~1cm) | Component (~ 1m) | Apparatus (~10m) | Factory (~100m, | Environment ~1000m)

Multi-level:

Product | Process | System

Bottleneck：

Multi-scale structure

Process | **Material**

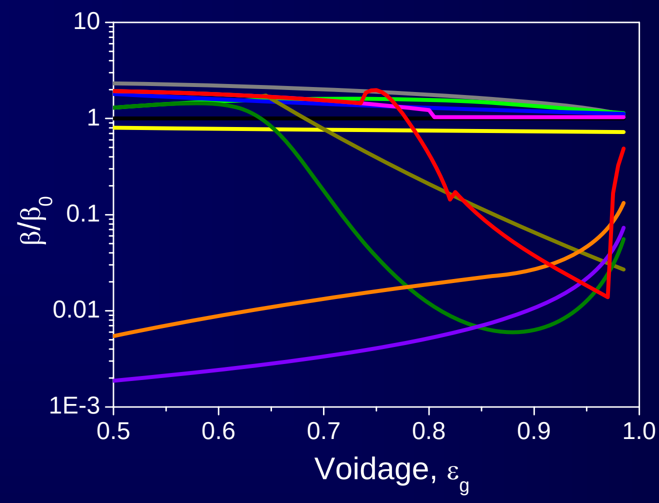
Challenge

In Physical Modeling

Poor predictability

Deviation between different methods

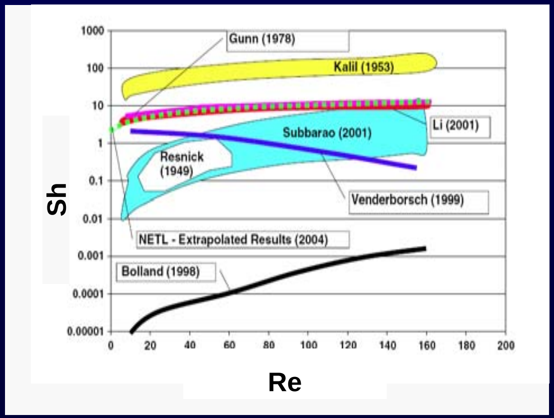
Drag Coefficient



3 ~ 4 orders of difference

+

Mass transfer



6 ~ 7 orders of difference

↓

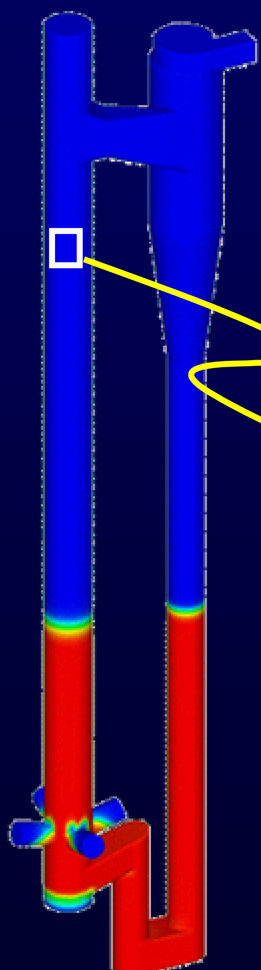
Reaction

Almost impossible

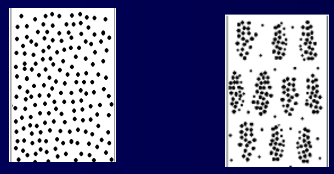
Process

EQUIPMENT SCALE

Axial and radial distribution

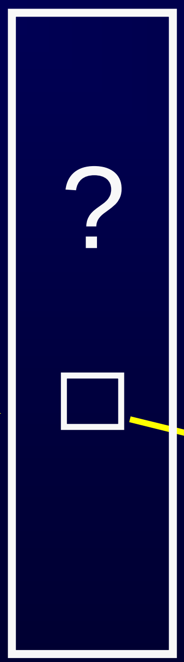


$\bar{C}_D$= 18.6 $\bar{C}_D$= 5.43



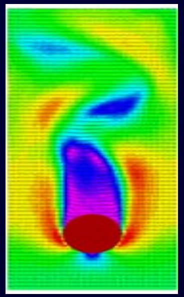
Critical influence on transport

MESO-SCALE



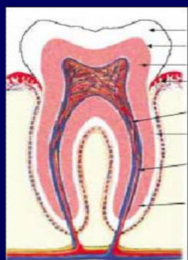
MICRO-SCALE

Flow, mass transfer and reaction around a particle



Material: *Hydroxyapatite*

MACRO

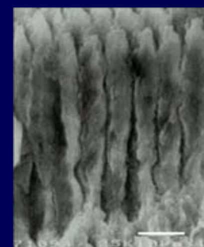


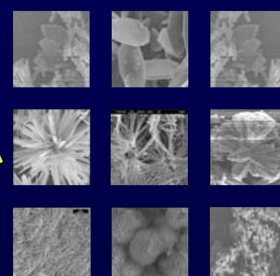
Tooth

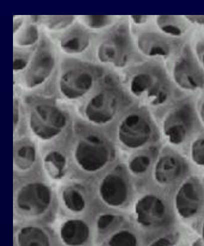
?

Bone

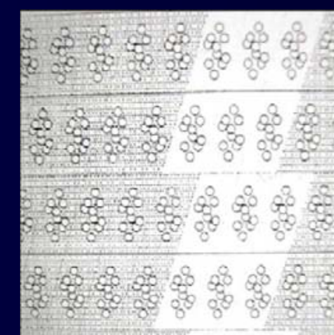
MESO ?







MICRO



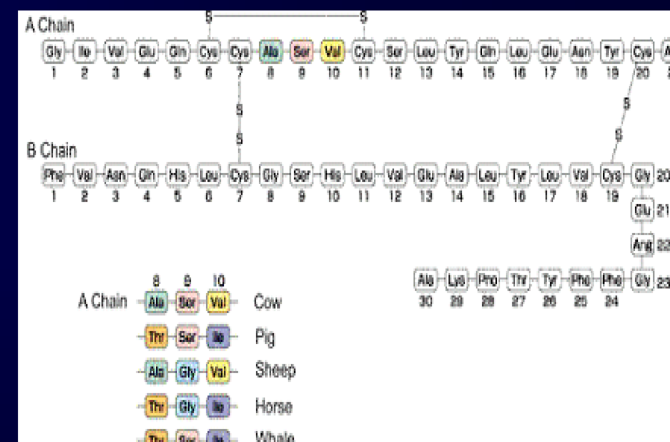
$Ca_5(OH)(PO_4)_3$

Material: ***Protein***

MACRO **MESO ?** **MICRO**

unfolding

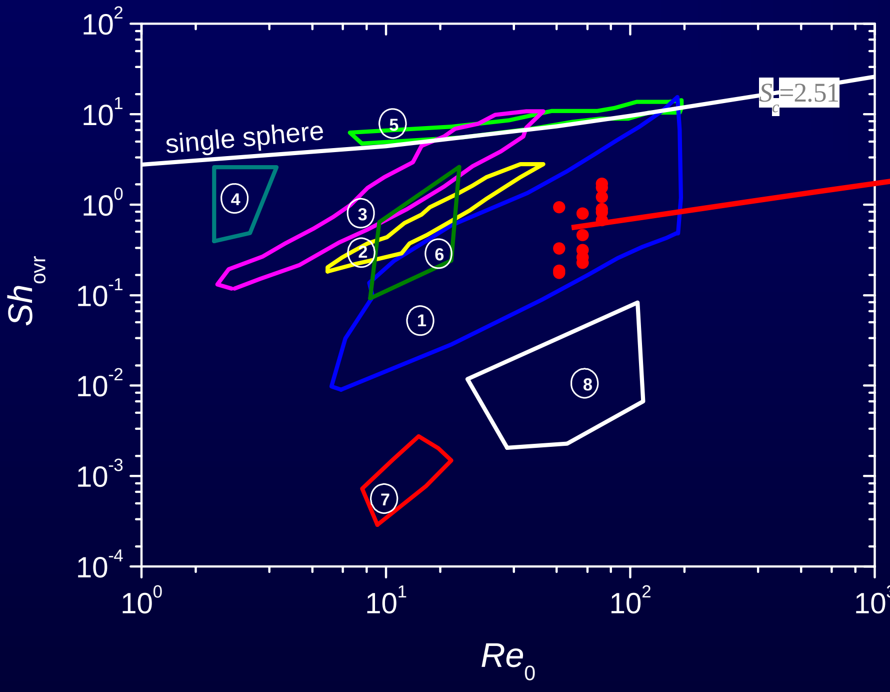
folding

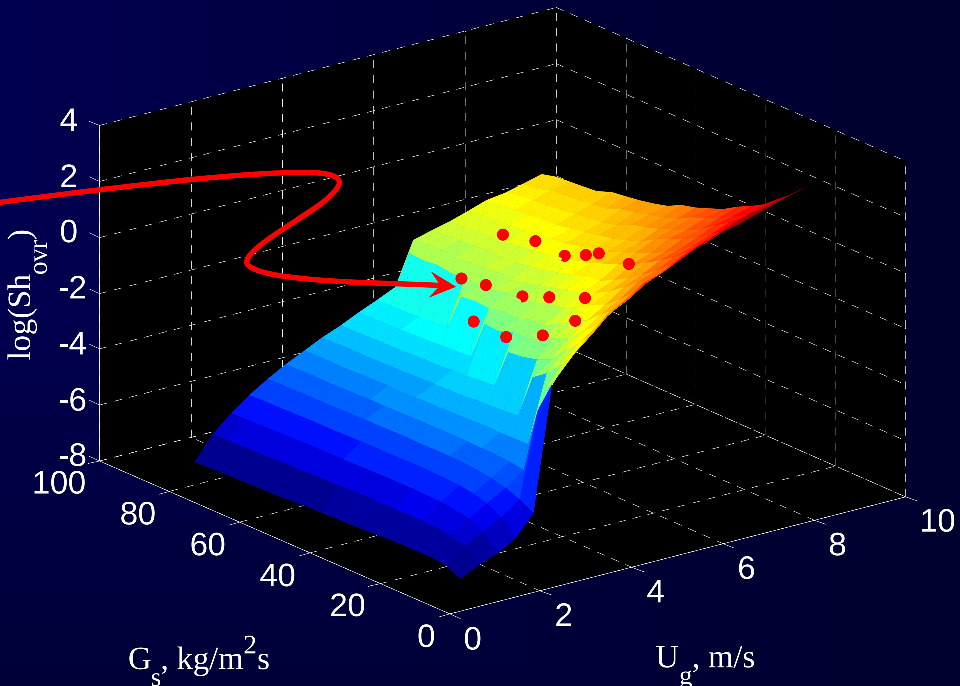


- Challenge in physical modeling is poor predictability

- Understanding of meso-scale structure is the bottleneck

Meso-scale structure is the key to achieve high predictability:



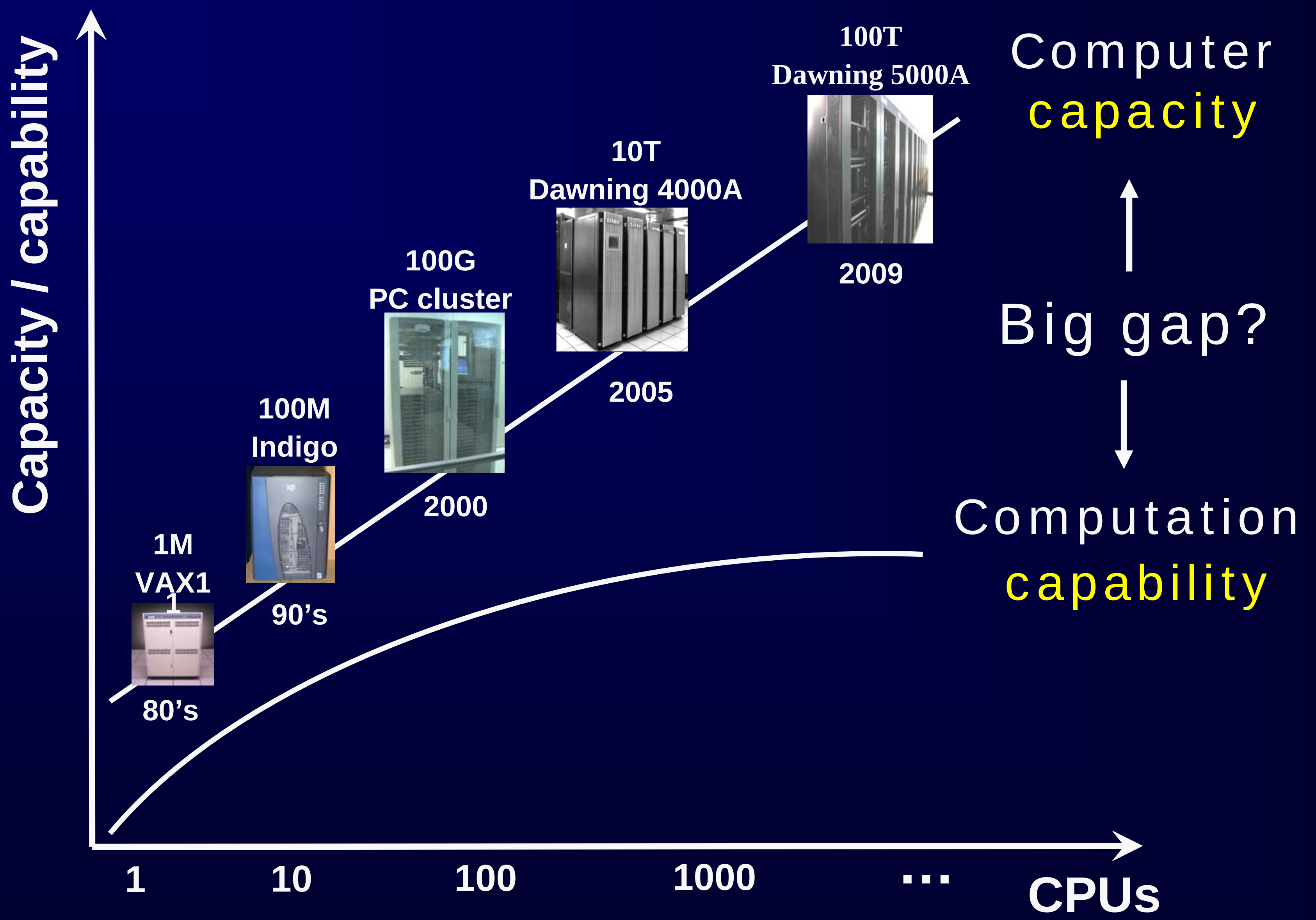


Dong et al, Chem. Eng. Sci., 63,2008, 2798-2823

Challenges

In Computation

High cost & low efficiency

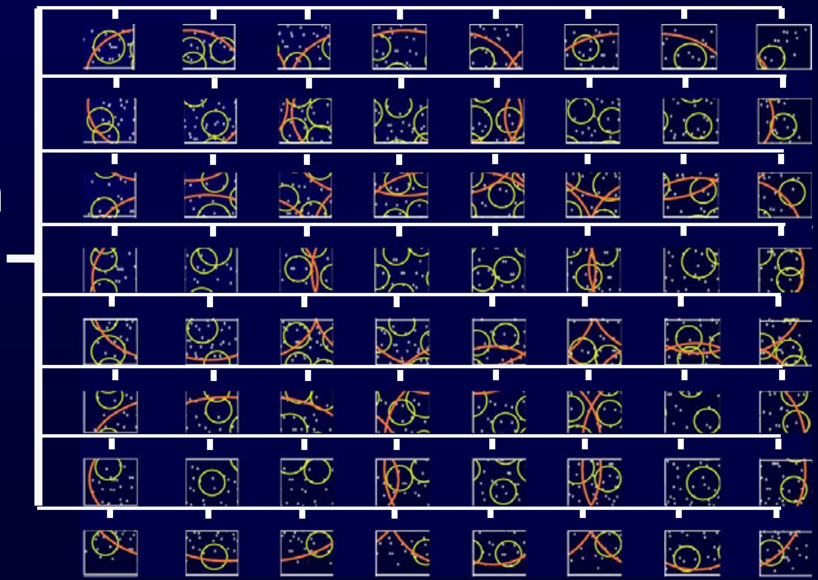

Capacity / capability
100T
Dawning 5000A
2009
10T
Dawning 4000A
2005
100G
PC cluster
2000
100M
Indigo
90's
1M
VAX1
1
80's
1
10
100
1000
...
CPUs
Computer
capacity
Big gap?
Computation
capability

Disparity
- **Structure of problems : Multi-scale**
- **Configuration of software : Diversity**
- **Architecture of computers: Single scale**

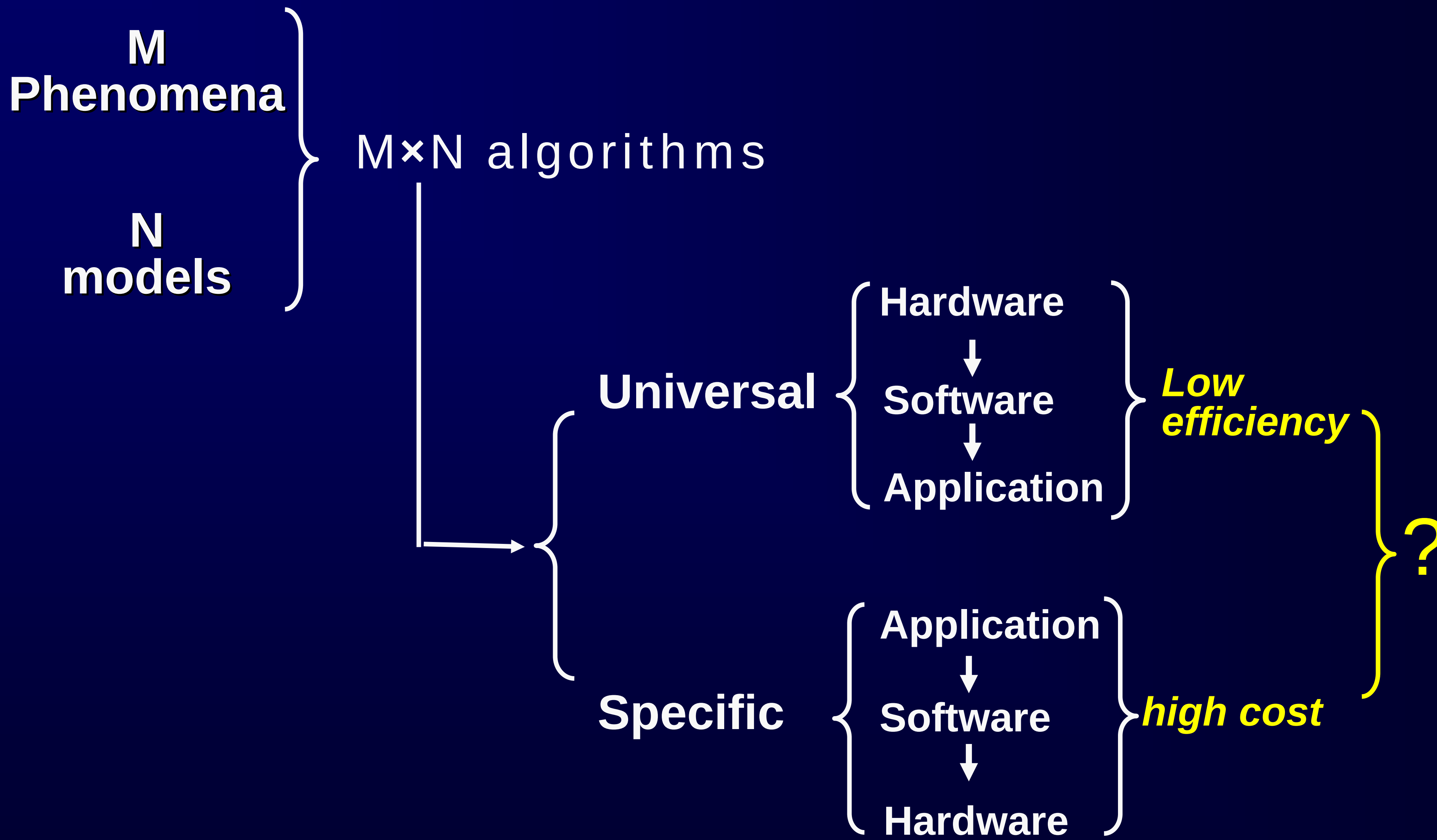
Single-scale architecture

Long-range correlation

Global communication



Diversity in algorithms



Strategy

In Physical Modeling

Varational Multi-scale Methodolgy

"Multi-scale science"

- **Glimm and Sharp, *SIAM News*, 1997**

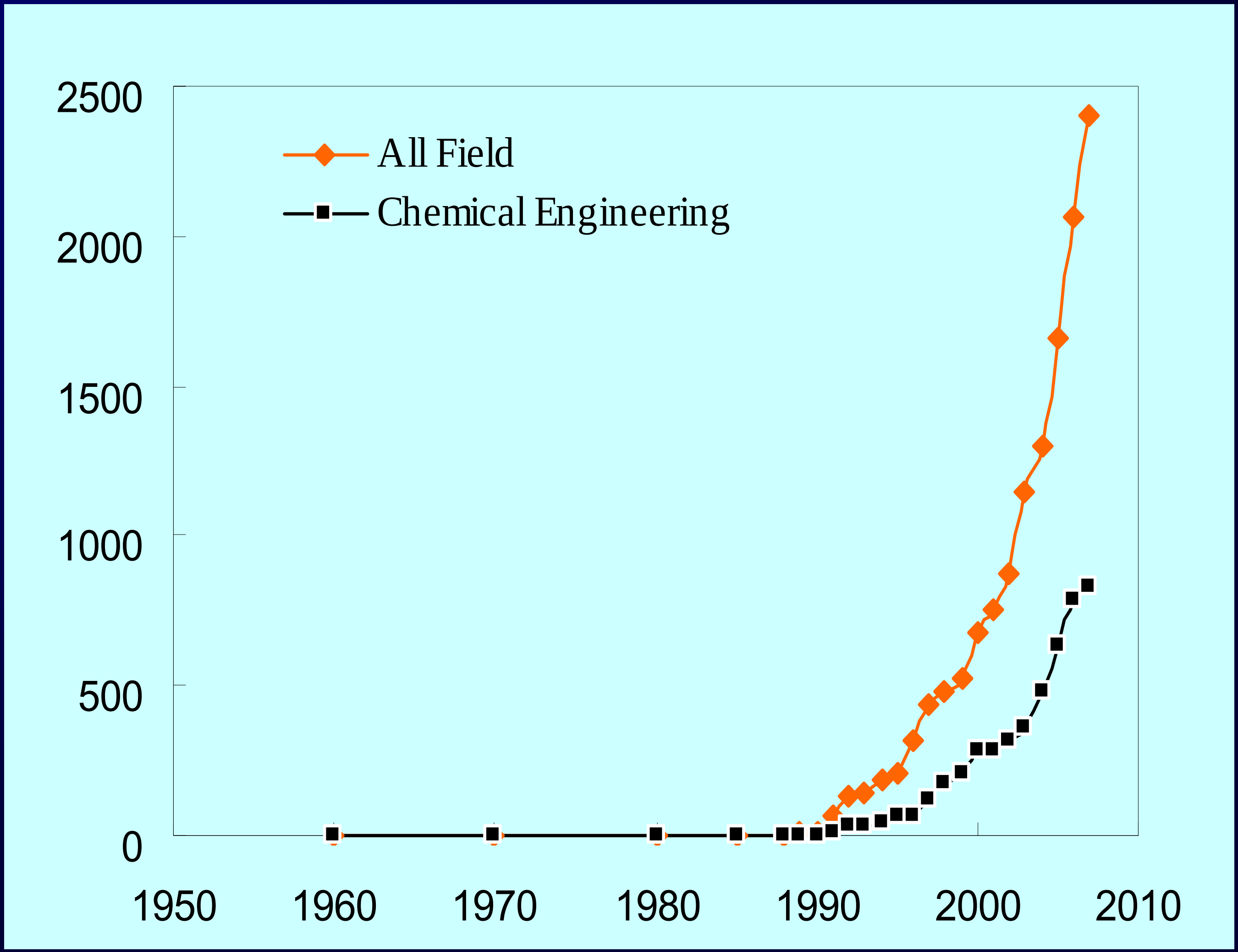
  Multi-scale Science

  – the challenge of 21st century

- **Krumhansl, *Material Science Forum*, 2000**

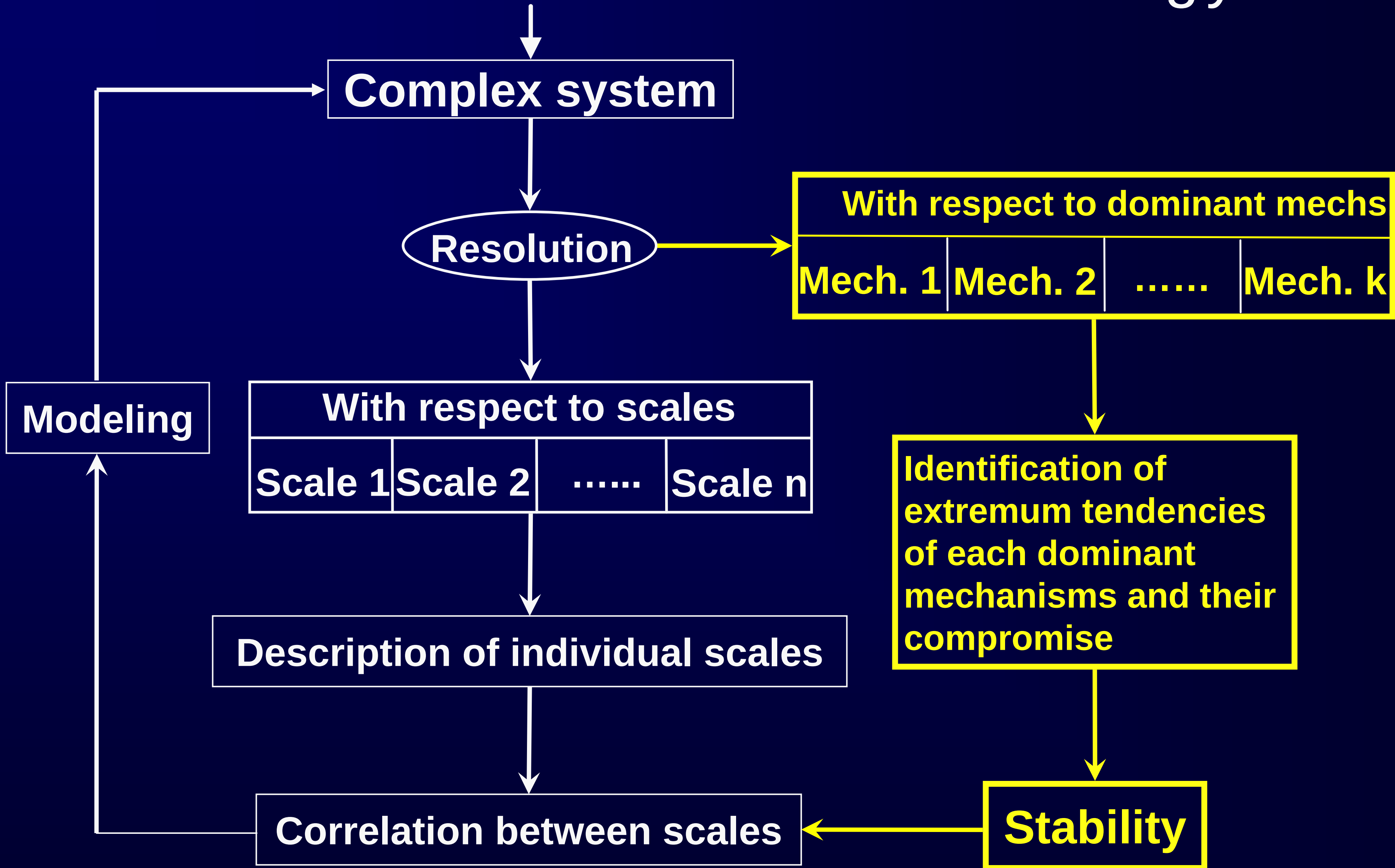
  Multi-scale Science

  – Material Science of 21st century



"Multi-scale" OR "Multiscale" within Keywords/Title/Abstract *http://isiknowledge.com/ on Nov. 14, 2008*

Variational multi-scale methodology



Stability criterion

- Equilibrium: *Max. Entropy*
- Non-Equilibrium
  - Linear: *Min. Entropy Production*
  - *Non-linear:* ?

Chemical Processes

Multi-scale Structure !

Complexity science

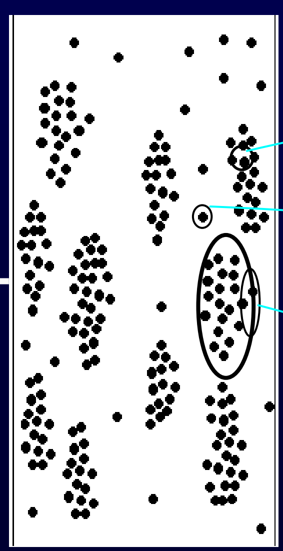
The 1st practice in gas/solid system

Insufficiency of conservation equations

Dense phase
- Gas velocity U_c
- Solid velocity U_{pc}
- Voidage ε_c
- Volume fraction f
- Cluster diameter d_{cl}

Dilute phase
- Gas velocity U_f
- Solid velocity U_{pf}
- Voidage ε_f

8 variables ⇒ **6 equations**



Particle-scale:

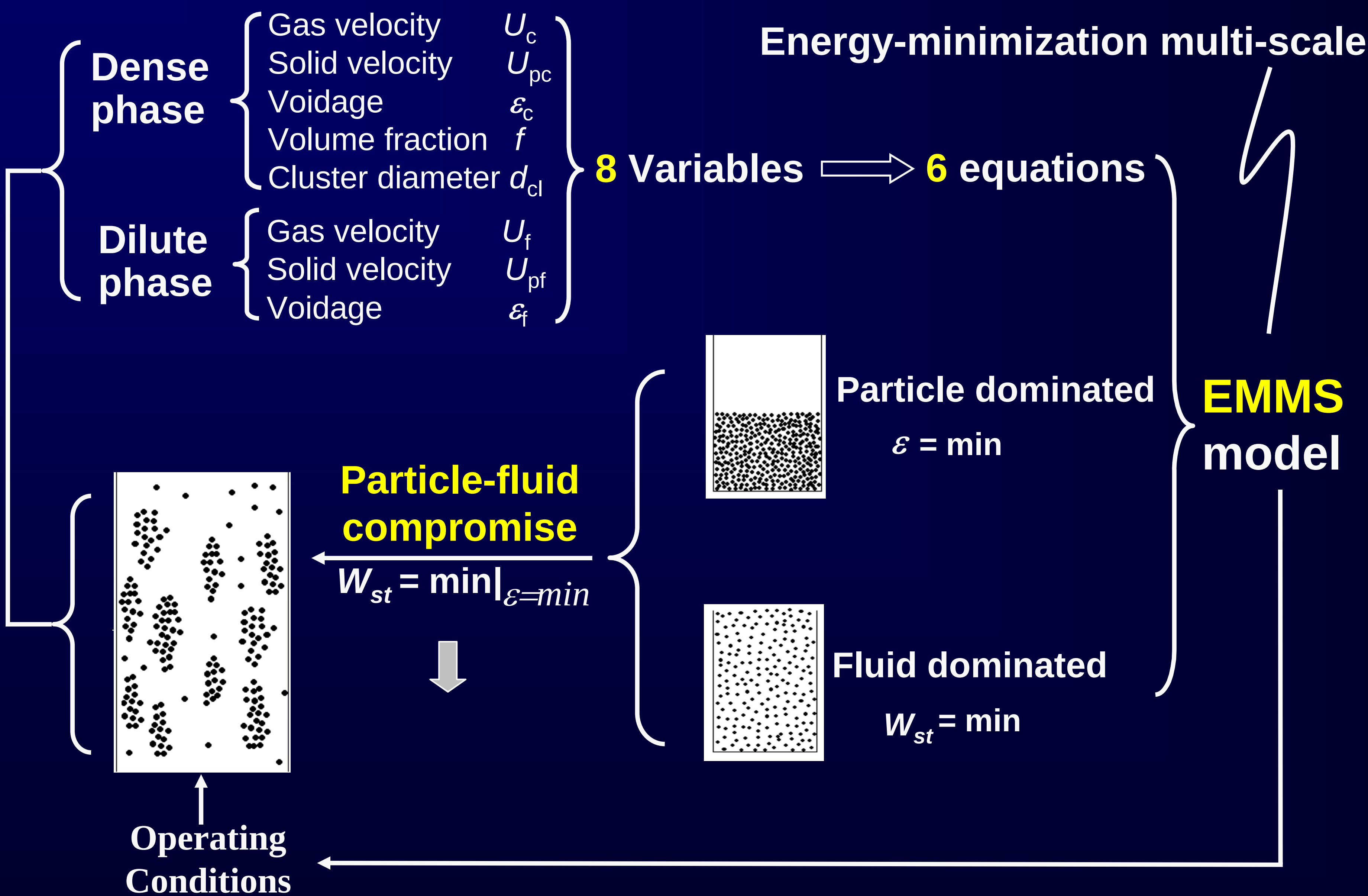
in dense-phase

in dilute-phase

Cluster-scale

Stability ?

Physical Concept of EMMS Model



Mathematical Formulation

To find : $\boldsymbol{X}=\{ U_{pc}, U_c, \varepsilon_c, f, d_{cl}, U_{pf}, U_f, \varepsilon_f \}$

Minimizing : $N_{st} = \dfrac{W_{st}}{(1-\varepsilon)\rho}$

s.t. $F_i(X)=0$

$$
\begin{cases}
F_1(\mathbf{X}) = m_c F_c f + m_i F_i - f(1-\varepsilon_c)(\rho_p - \rho_f)g = 0 \\
F_2(\mathbf{X}) = m_f F_f - (1-\varepsilon_f)(\rho_p - \rho_f)g = 0 \\
F_3(\mathbf{X}) = m_f F_f + m_i F_i/(1-f) - m_c F_c = 0 \\
F_4(\mathbf{X}) = U_p - U_{pf}(1-f) - U_{pc} f = 0 \\
F_5(\mathbf{X}) = U_g - U_f(1-f) - U_c f = 0 \\
F_6(\mathbf{X}) = d_{cl} - \dfrac{d_p \left[\dfrac{U_p}{1-\varepsilon_{\max}} - (U_{mf} + \dfrac{U_p \varepsilon_{mf}}{1-\varepsilon_{mf}}) \right] \cdot g}{N_{st} \dfrac{\rho_p}{\rho_p - \rho_f} - (U_{mf} + \dfrac{U_p \varepsilon_{mf}}{1-\varepsilon_{mf}}) \cdot g} = 0
\end{cases}
$$

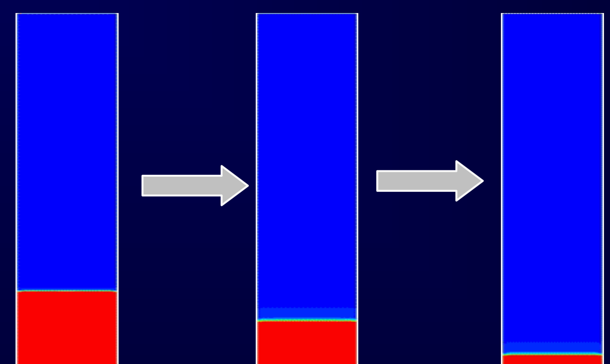
Previously:

- Local structural parameters

8 variables

Gas velocity	U_c
Solid velocity	U_{pc}
Voidage	ε_c
Volume fraction	f
Cluster diameter	d_{cl}
Gas velocity	U_f
Solid velocity	U_{pf}
Voidage	ε_f

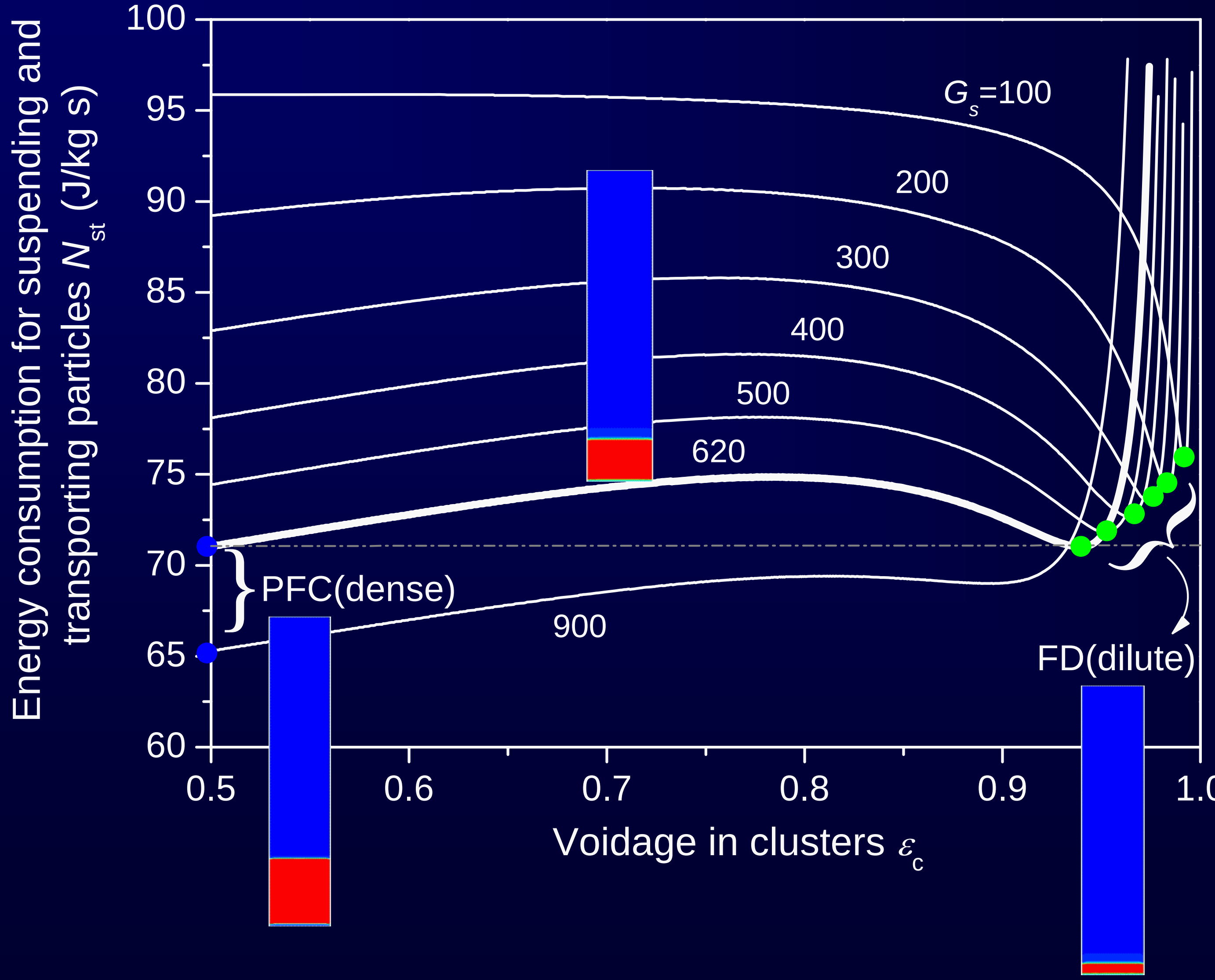
- Regime diagram



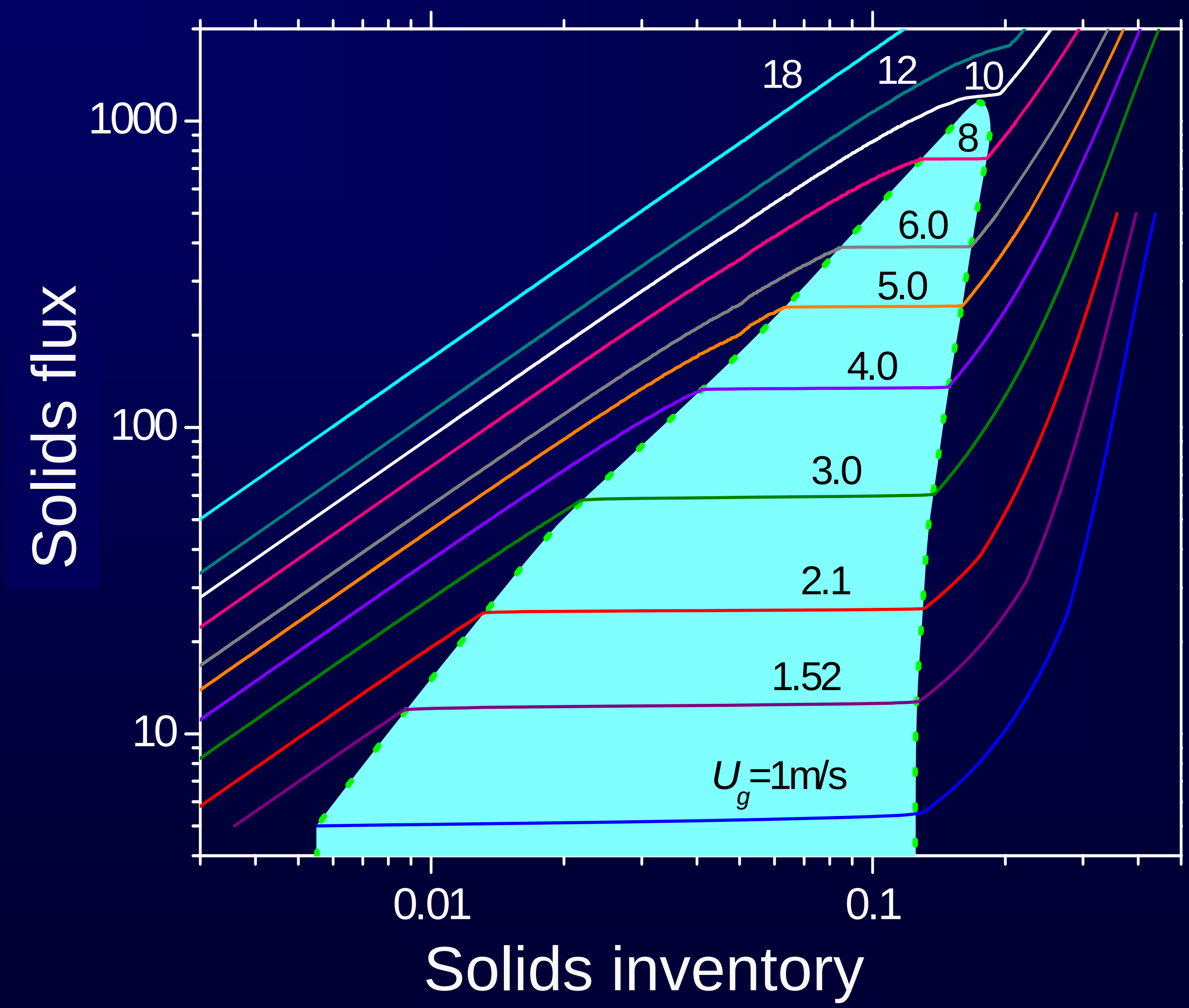
- Radial and axial distributions

Prediction of chocking

Ge&Li, Chem. Eng. Sci. 2002, Vol. 56; Wang et al Chem. Eng. Sci. 2007 Vol. 62



Intrinsic flow regime predicted by EMMS



http://pevrc.ipe.ac.cn/emms/emmsmodel.php3

Online service

http://pevrc.ipe.ac.cn/emms/emmsmodel.php3

EMMS Flow Prediction Tool

Introduction:

- This is a flow prediction tool for CFB risers based on the EMMS model proposed by Jinghai Li and Mooson Kwauk. The gas-solid system here is resolved into a dense phase in clusters and a surrounding dilute phase, the phase-averaged concentrations and velociti ... and dense phase fraction, can be calculated from given ma...

Please specify your system:

Sketch of Model

DESCRIPTION	SYMBOL	UNIT	VALUE	
fluid density	ρ_f	kg/m^3	user input (ρf>0)	or CHOOSE
fluid dynamic viscosity	μ	kg/m.s	user input (μ>0)	or CHOOSE
#1 particle diameter	d_p	m	user input (dp>0)	
#2 riser inner diameter	d_t	m	user input (dt>0)	
minimum fluidization voidage	ε_{mf}		user input (0<εmf<1)	
particle real density	ρ_p	kg/m^3	user input (ρp>0)	or CHOOSE
solids flow rate	G_s	kg/m^2.s	user input (Gs>0)	
superficial fluid velocity	U_g	m/s	user input (Ug>0)	

Please select the way of attaining the results from this tool:

- ◉ Send the results to your E-mail:
- ○ Show the results in the current window.

submit reset

Discrete simulation & verification

N_{st} = min ?

- Whether or not ?
- If yes, why?

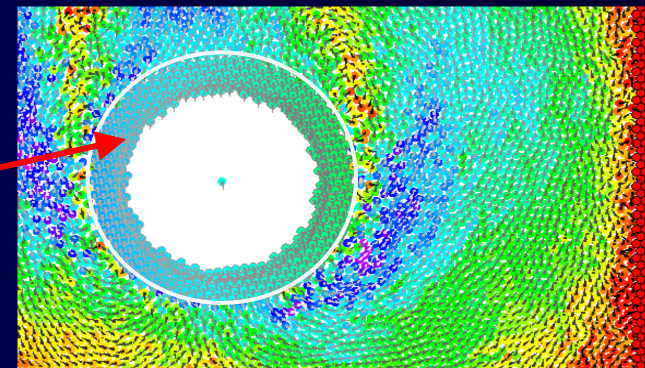
↓

Pseudo-Particle

- Micro-scale description
- Macro-scale phenomena

Macro-scale Pseudo-Particle Modeling

Numerical Operators → "Interactions" between "Particles"



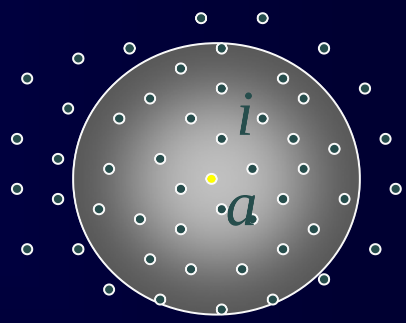
Physical
- **Particles**
- **Fluid → Pseudo-particles**

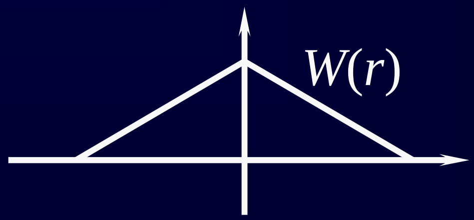
Mathematical

$$\dot{\boldsymbol{V}} = \boldsymbol{g} - k'\nabla\rho + \nu\Delta\boldsymbol{V}$$

$$\nabla\rho\,\big|_a = \sum_i \frac{W_{ai}}{r_{ai}^2}\boldsymbol{r}_{ai}$$

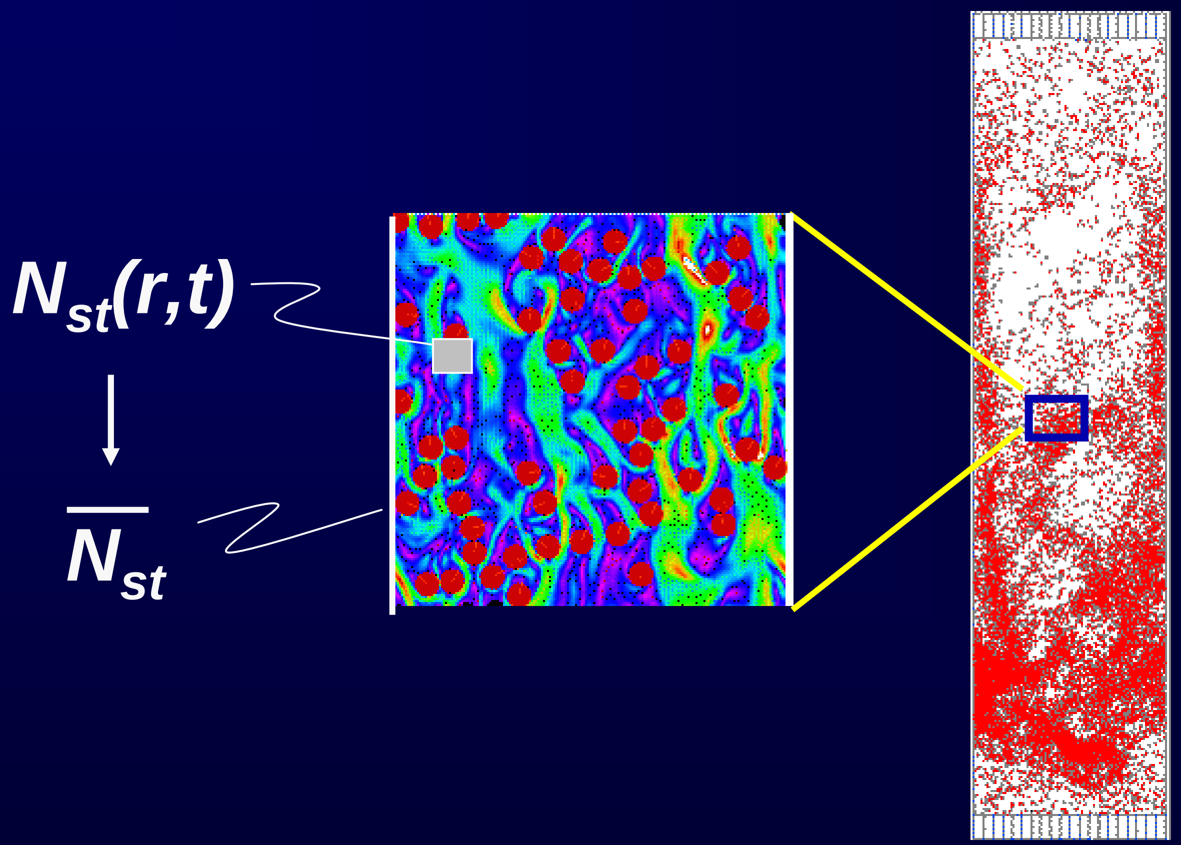
$$\Delta\boldsymbol{V}\,\big|_{\boldsymbol{a}} = \frac{2}{\rho_{\mathrm{m}}}\sum_i \frac{\boldsymbol{V}_{ia}}{r_{ai}^2} W_{ai}$$



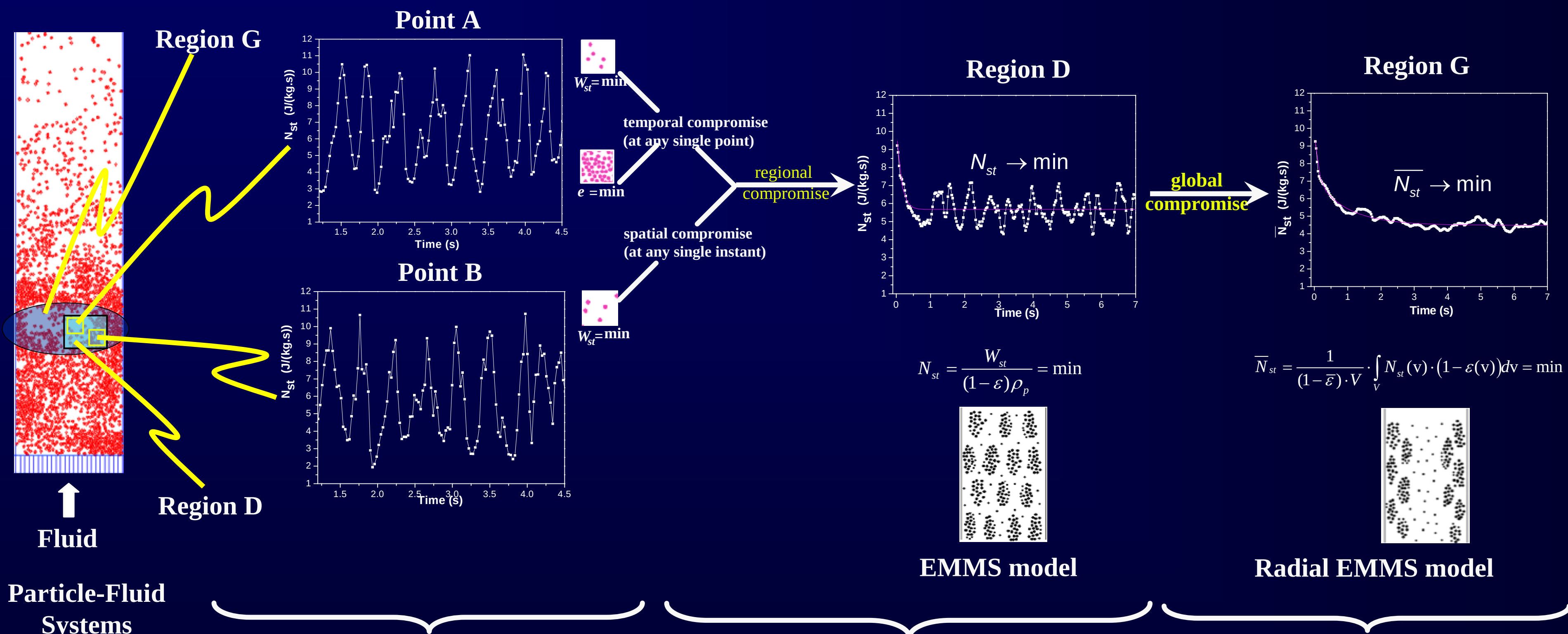


Ge & Li: CFB5, 1996; Chem. Eng. Sci., 58, 2003, 1565; Powder Tech. 137:99

Generating meso- and micro-scale structures with micro-phenomena:



$N_{st} \rightarrow$ min was verified in 2004



Local (micro-scale) structure:
Point A & B

Meso-scale structure:
Region D

Global (macro-scale) structure:
Region G

Li et al., Chem. Eng. Sci. Vol.59 , 2004 , 1687 ~ 1700

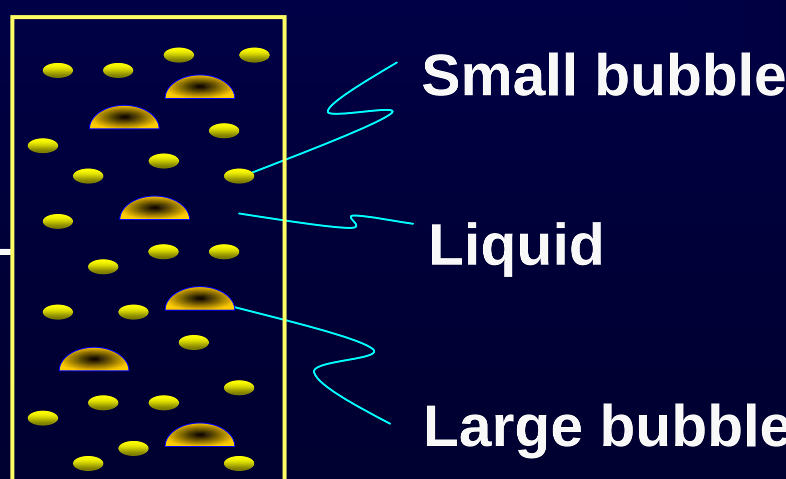
The 2^{nd} practice in gas/liquid system

Insufficiency of conservation equations:

Small bubbles
- Gas velocity $U_{g,S}$
- Volume fraction f_S
- Bubble diameter d_S

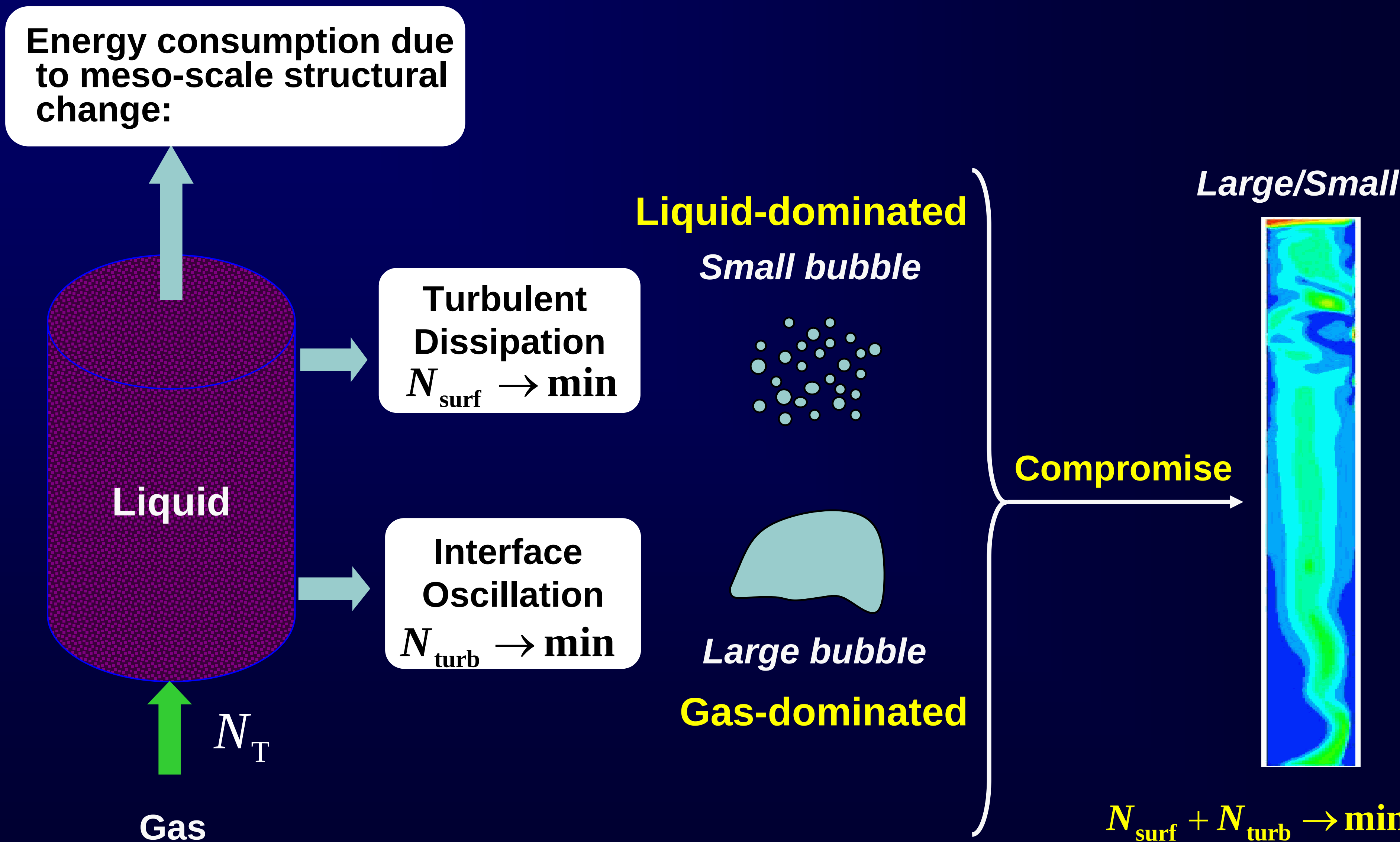
Large bubbles
- Gas velocity $U_{g,L}$
- Volume fraction f_L
- Bubble diameter d_L

6 Variables ⇨ 3 equations



Stability ?

Path of energy transfer and dissipation



Zhao, Ge & Li, Chem. Eng. Sci., 2007

Physical Model

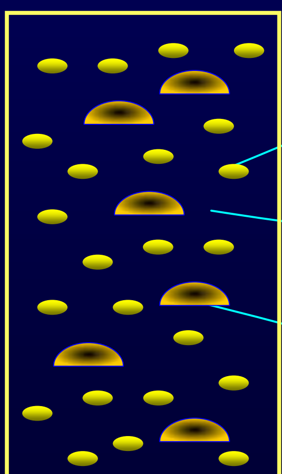
Small bubbles
- Gas velocity $U_{g,S}$
- Volume fraction f_S
- Bubble diameter d_S

Large bubbles
- Gas velocity $U_{g,L}$
- Volume fraction f_L
- Bubble diameter d_L

6 Variables ⇨ **3 equations**

Dual-bubble-size model

DBS model



Small bubble

Liquid

Large bubble

Compromise between dominant mechanisms

?

between scales

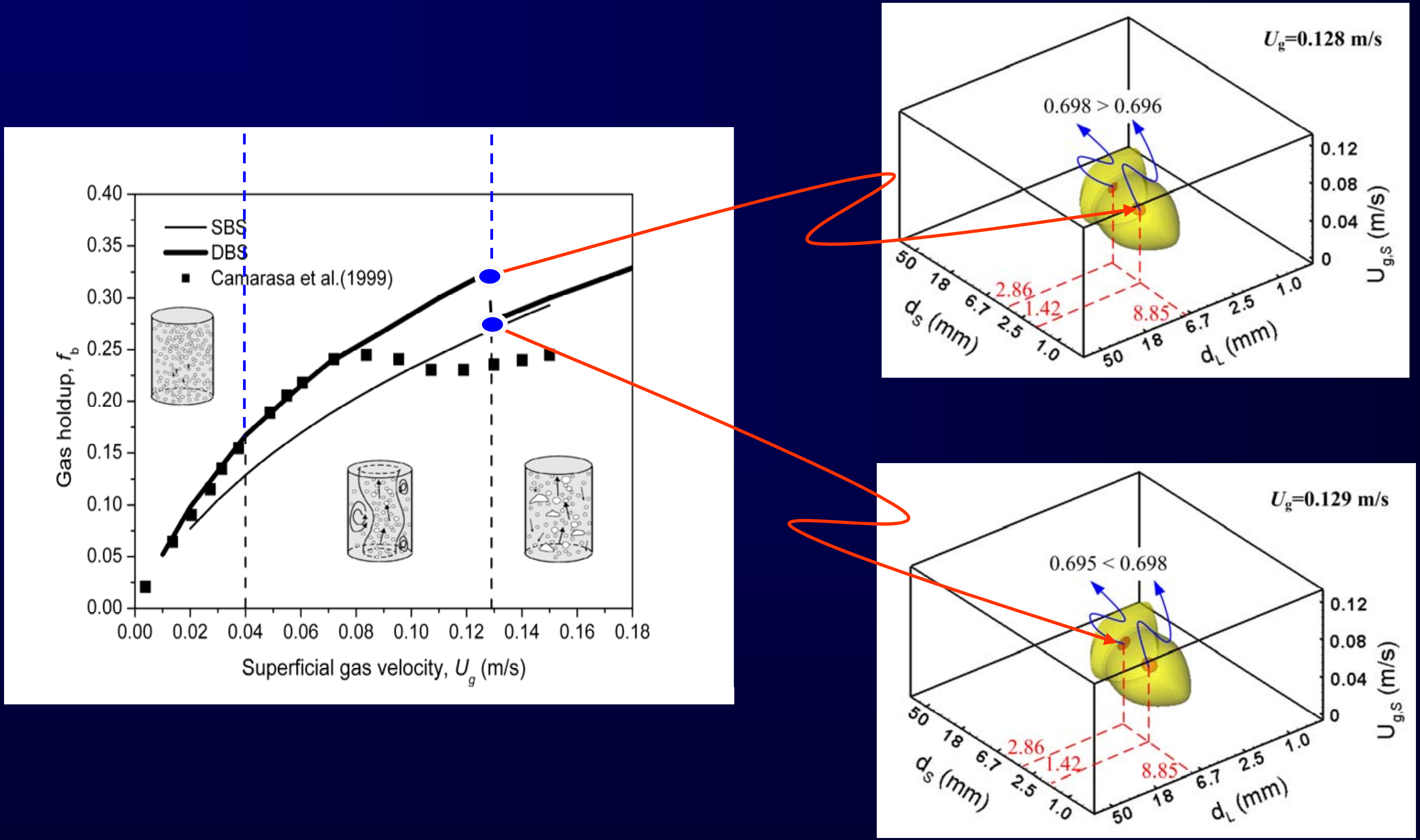
⇩

Stability Condition:

$$N_{\mathrm{surf,S+L}} + N_{\mathrm{turb}} \rightarrow \min.$$

Operating Conditions

The jump change of flow structure

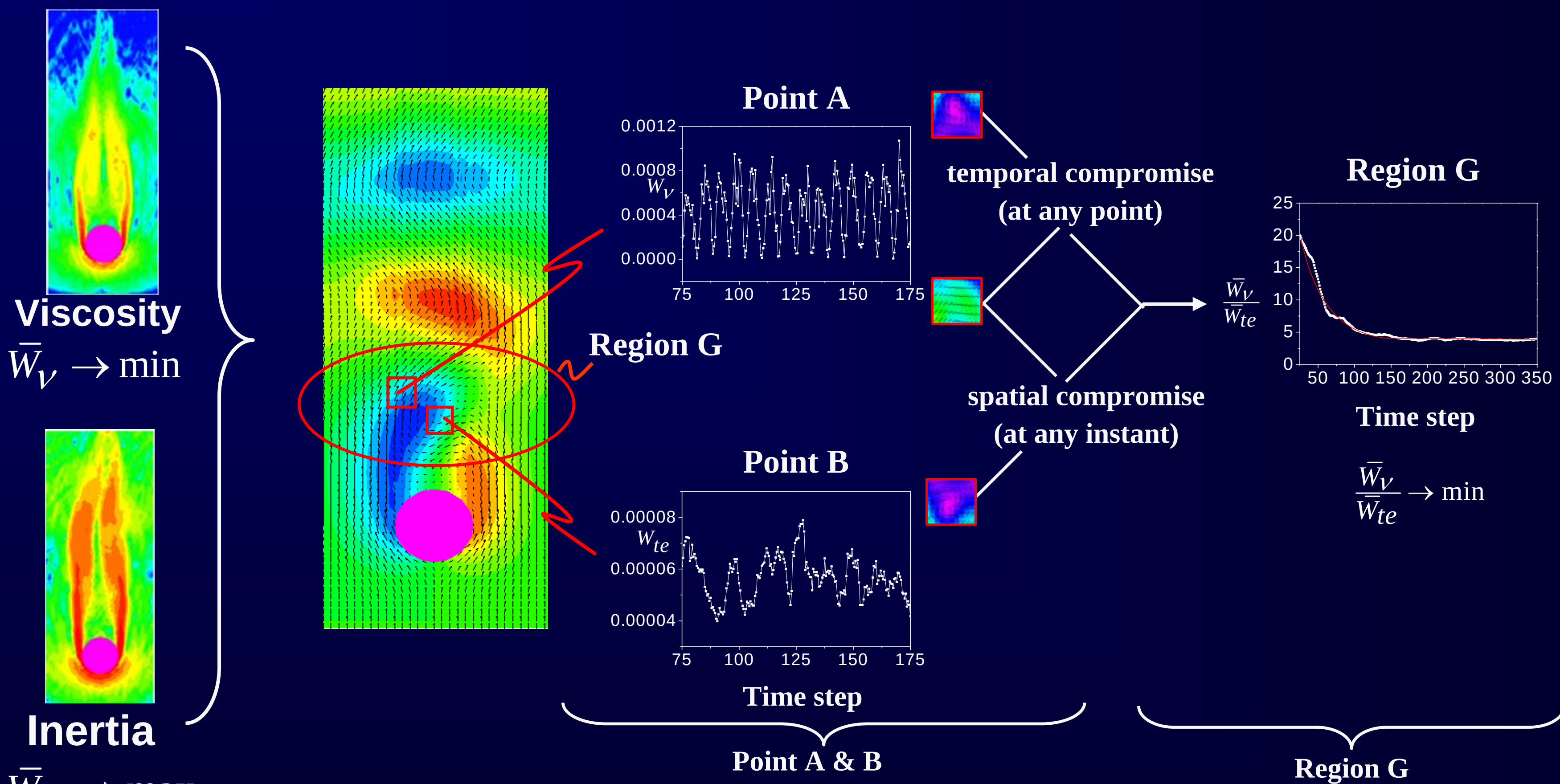


Yang, Chen, Zhao, Ge & Li, Chem. Eng. Sci., 2007

Extension to more systems for generalization

Extension 3: Turbulent Flow

Compromise between Viscosity and Inertia

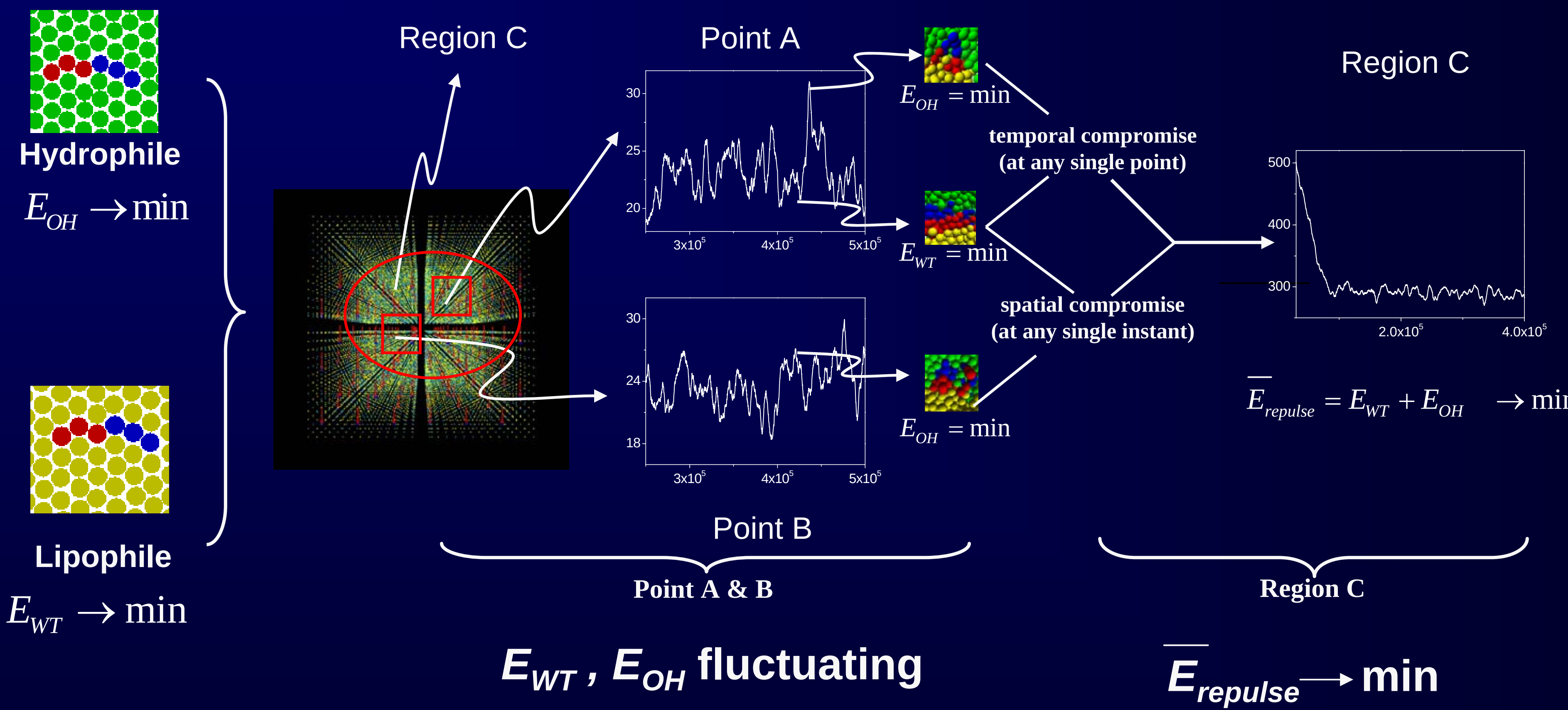


$\overline{W}_v$, $\overline{W}_{te}$ fluctuating

$\overline{\overline{W}_v / \overline{W}_{te}} \rightarrow$ min

Extension 4: Microemulsion

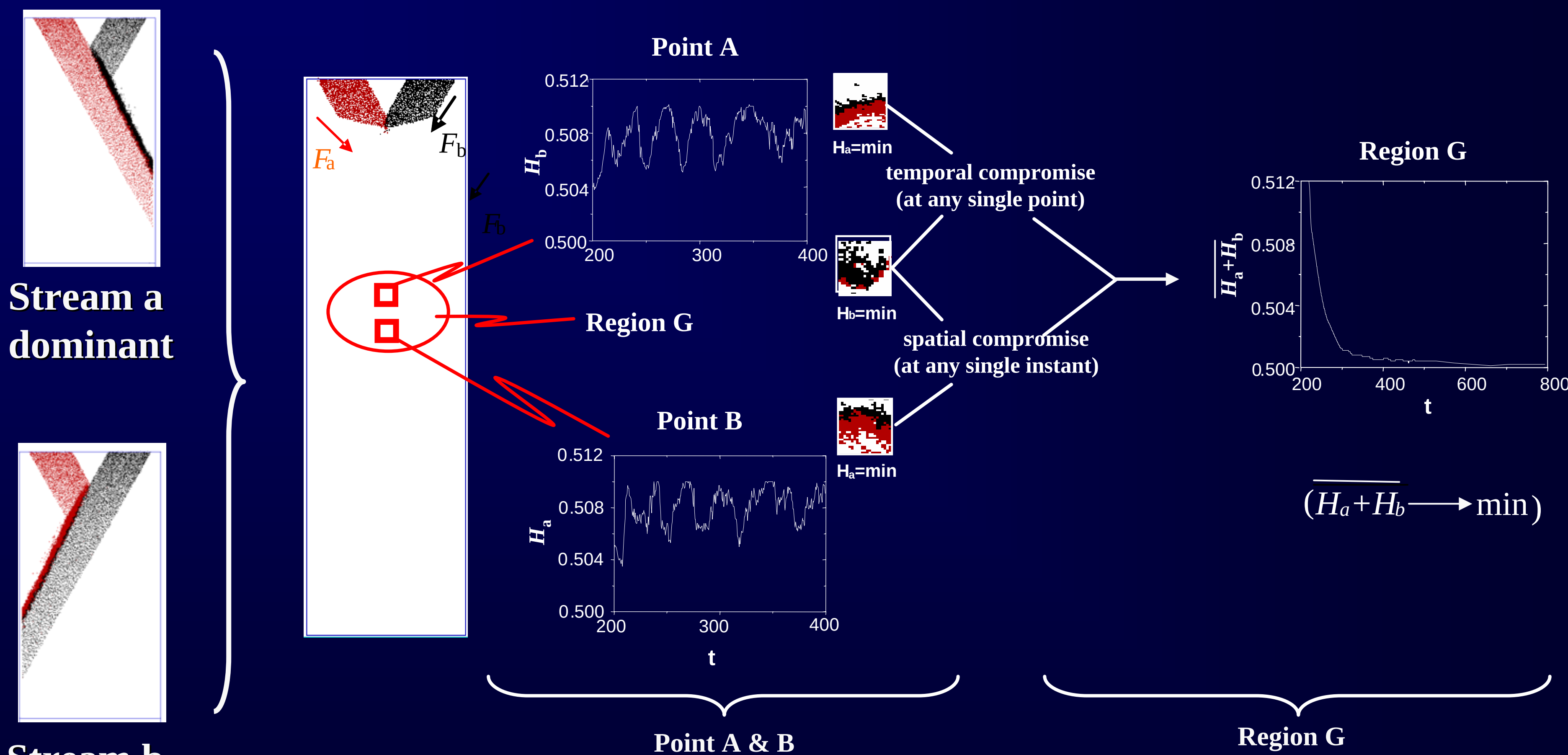
Compromise between Hydrophile and Lipophile



H: Hydrophile group (red) **T**: Lipophile group (blue) **W**: Water (green) **O**: Oil (yellow)

Extension 5: Granular Flow

Compromise Between Two Streams of Granular Flow

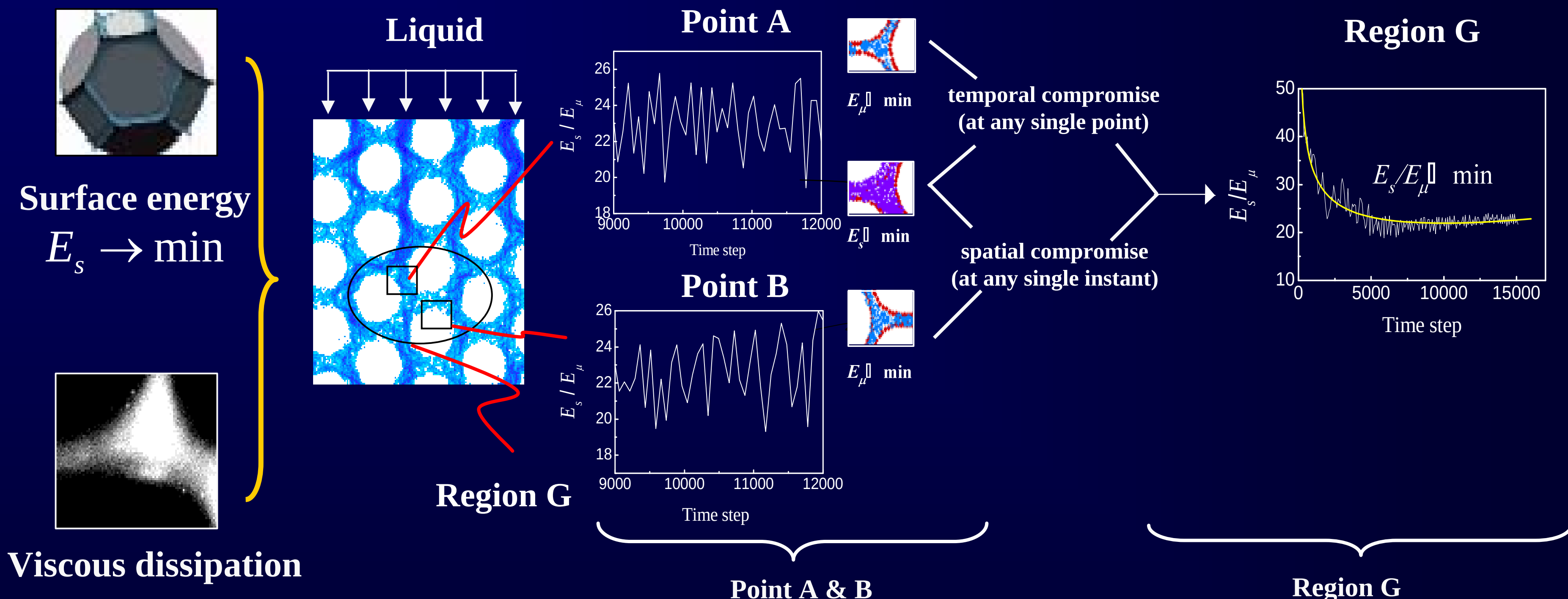


H_a , H_b fluctuating

$\overline{H_a + H_b} \rightarrow \min$

Extension 6: Foam Drainage

Compromise Between Surface Energy and Viscosity



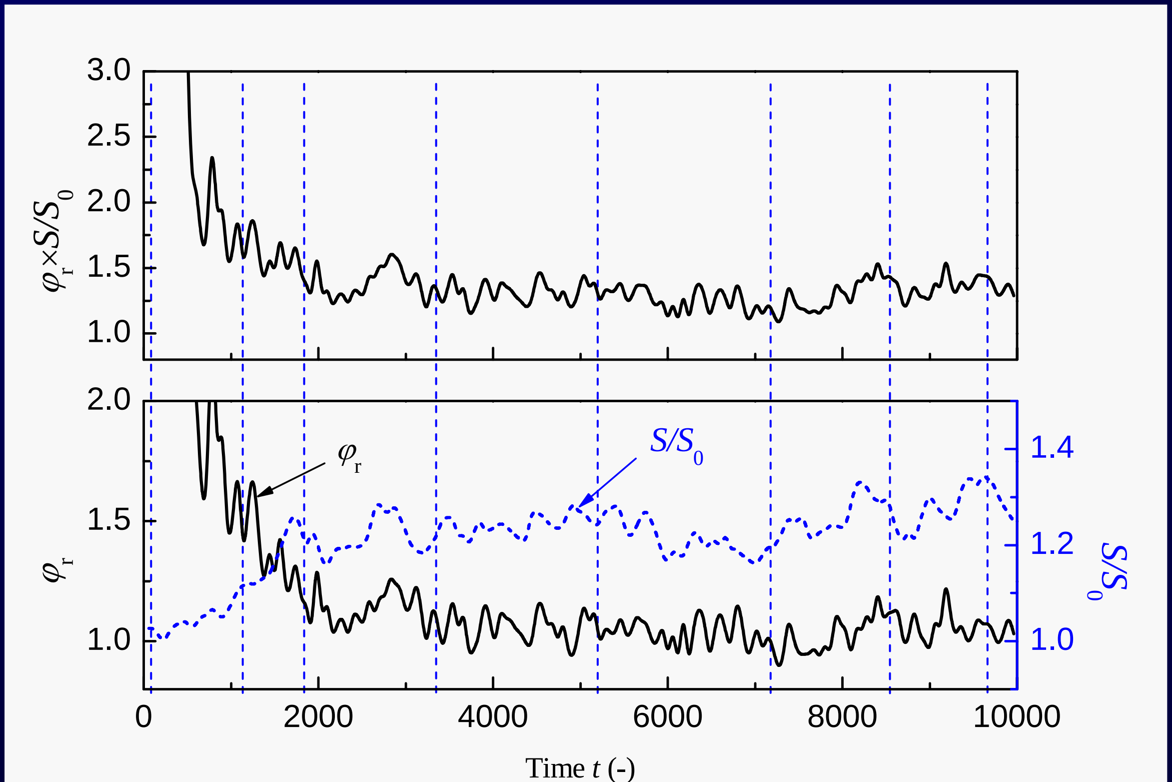
E_s , E_μ fluctuating

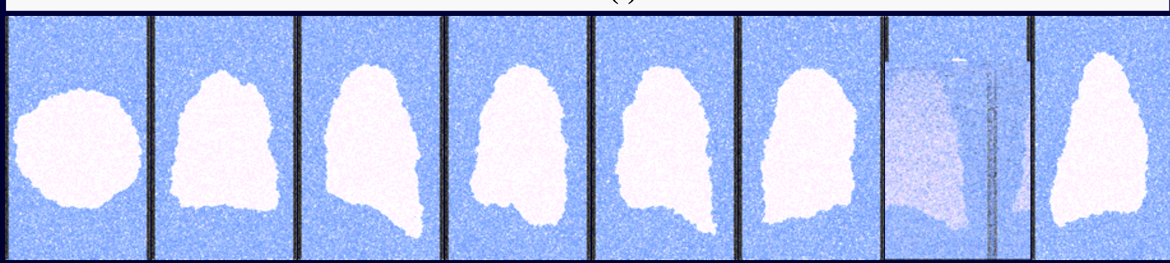
$\overline{E_s/E_\mu} \rightarrow \min$

Extension 7: Nano Gas-liquid Flow

Compromise Between Interfacial Potential and Viscosity

a b c d e f g h





a b c d e f g h

φ_r	The "cost–benefit" ratio of the energy transportation.

$$\varphi_r = \frac{F\int_A V_m(A)dA \Big/ \int_A dA}{\frac{1}{2}\int_A \rho_m(A)V_m^3(A)dA}$$

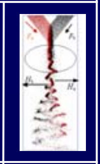
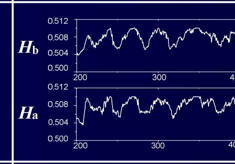
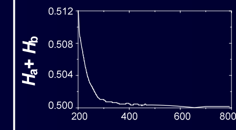
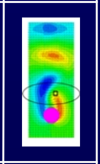
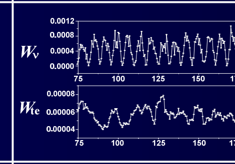
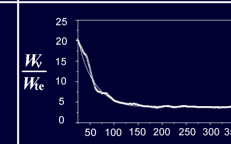
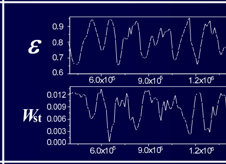
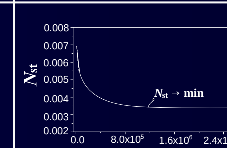
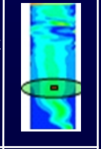
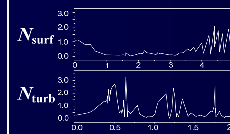
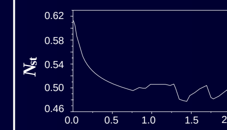
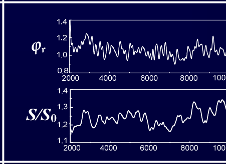
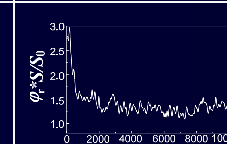
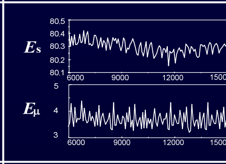
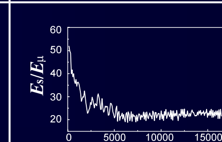
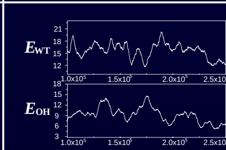
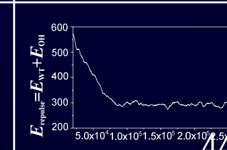
S	Interfacial area

Compromise

$$\varphi_r S \to \min$$

Summary:

Ge et al Chem. Eng. Sci. 2007

1. Systems		2. Dominant mechanisms: Compromise	2. Dominant mechanisms: Definition	3. Local extremum: existence	3. Local extremum: indication	4. Global extremum: existence	4. Global extremum: indication
Cross flow of granular materials		$(H_a = \min)\|_{H_b=\min}$	H_a --- potential a H_b --- potential b	No		Yes	
Turbulent flow		$(\overline{W}_\nu = \min)\|_{\overline{W}_{te}=\max}$	$\overline{W}_\nu$ --- viscous dissipation $\overline{W}_{te}$ --- turbulent dissipation	No		Yes	
Gas-solid system		$(W_{st} = \min)_{\varepsilon=\min}$	W_{st} --- volume specific energy consumption for transporting and suspending particles ε--- local voidage of the identified area	No		Yes	
Turbulent gas-liquid flow		$(N_{turb} = \min)\|_{N_{surf}=\min}$	N_{turb} --- dissipation liquid in the turbulent N_{surf} --- surface dissipation	No		Yes	
Nano gas-liquid pipe flow		$(\varphi_r = \min)_{S=\min}$	φ_r --- dissipation associated with the transportation of unit amount of kinetic energy across unit length S --- surface energy in the system	No		Yes	
Foam drainage		$(E_s = \min)\|_{E_\mu=\min}$	E_s --- surface energy E_μ --- viscous dissipation	No		Yes	
Emulsion		$(E_{WT} = \min)\|_{E_{OH}=\min}$	E_{WT} --- lipophilic potential E_{OH} --- hydrophilic potential	No		Yes	

Compromise between dominant mechanisms

↓

Dependence between scales

↓

Gas-solid flow

Gas-liquid flow

Turbulent flow

Granular flow

Foam drainage

Microemulsion

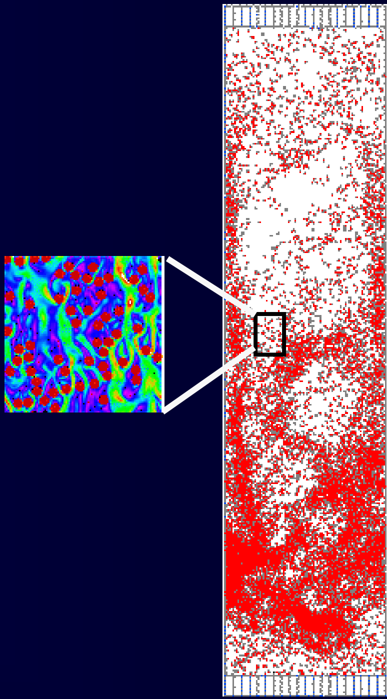
Nano flow

Stability:

{Extremum tendency of mechanism 1}

{Extremum tendency of mechanism 2}

←



↓

Generality?

Mathematical model of complex systems

$$X = \{ x_1, x_2, \ldots\ldots, x_n \}$$

$$\min \begin{pmatrix} E_j(X) \\ \vdots \\ E_k(X) \end{pmatrix}$$

$$s.t.\ \ F_i(X)=0,\ \ i=1, 2, \ldots, m$$

Multi-objective variational problem

J. Li et al., Chem. Eng. Sci., 2003, 58, 521- 535

Strategy

in Computation

Multi-scale structure { **Problems** / **Software** / **Hardware** } **Similarity**

New computation approach

Different problems in engineering

↓

Common nature

- Multi-scale
- Discrete

Physical model

$$X = \{x_1, x_2, \ldots\ldots, x_n\}$$

$$\min \begin{pmatrix} E_j(X) \\ \vdots \\ E_k(X) \end{pmatrix}$$

$$s.t.\ \ F_i(X)=0,\ \ i=1, 2, \ldots, m$$

Multi-objective variation

→ Software

↓

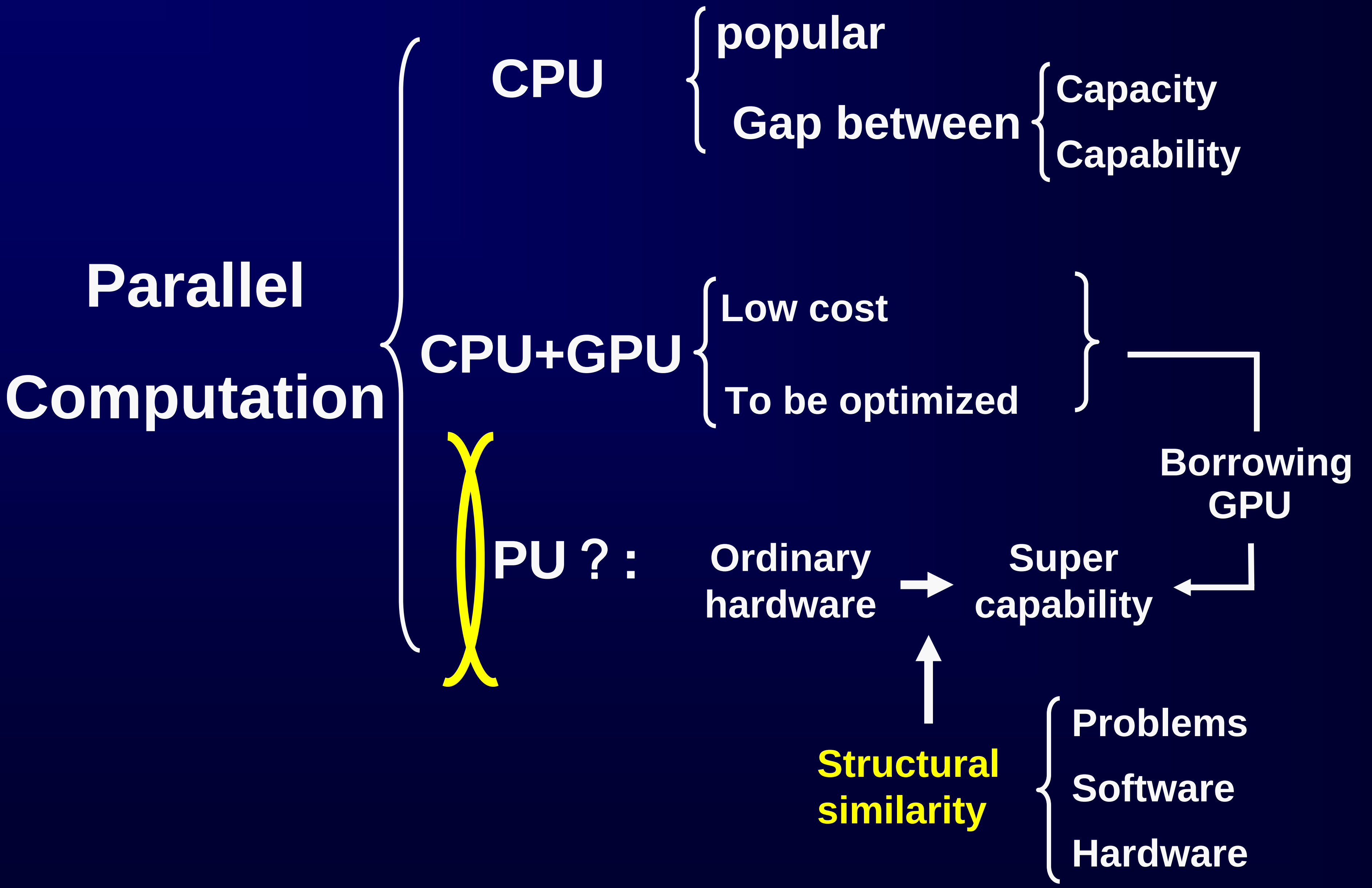
Computer

- Low cost
- High efficiency
- Generality

Two different strategies:

Chemical engineers
↓
Computer scientists → Computer → software → computation

Chemical engineers → physical models → software → computer → computation
↑
Computer scientists


Parallel
Computation
CPU
popular
Gap between
Capacity
Capability
CPU+GPU
Low cost
To be optimized
Borrowing
GPU
PU ? :
Ordinary
hardware
Super
capability
Structural
similarity
Problems
Software
Hardware

Macro

Meso

Variational multi-scale → CPU

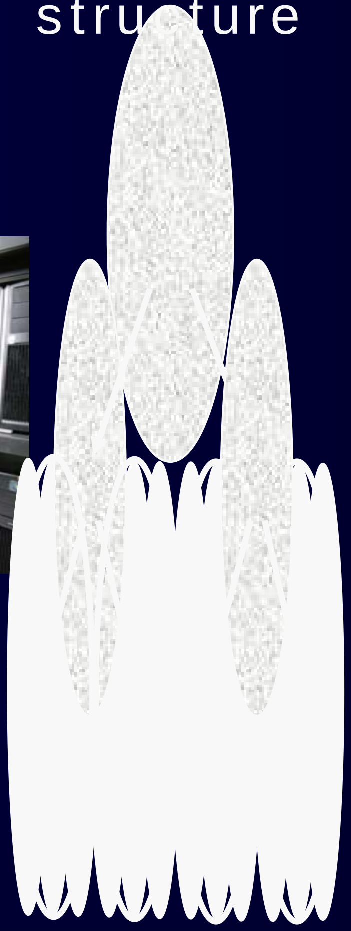
Computer structure

Physical structure

↕

Software structure

Lower scale variables



Micro: Pseuo-particle → GPU

Multi-scale Discrete Parallel Computation

Progresses

The 1.0 Peta flops system

Cooperation
- **Lenovo Co. /NV, 200T, Cuda**
- **Dawning Co./AMD, 200T, Brook/CAL**

150T / AMD built by IPE

Upgrading 120T → 450T

→ **1P flops**

200T(Dawning)

200T(Lenovo)

150T(IPE)

450T(IPE)

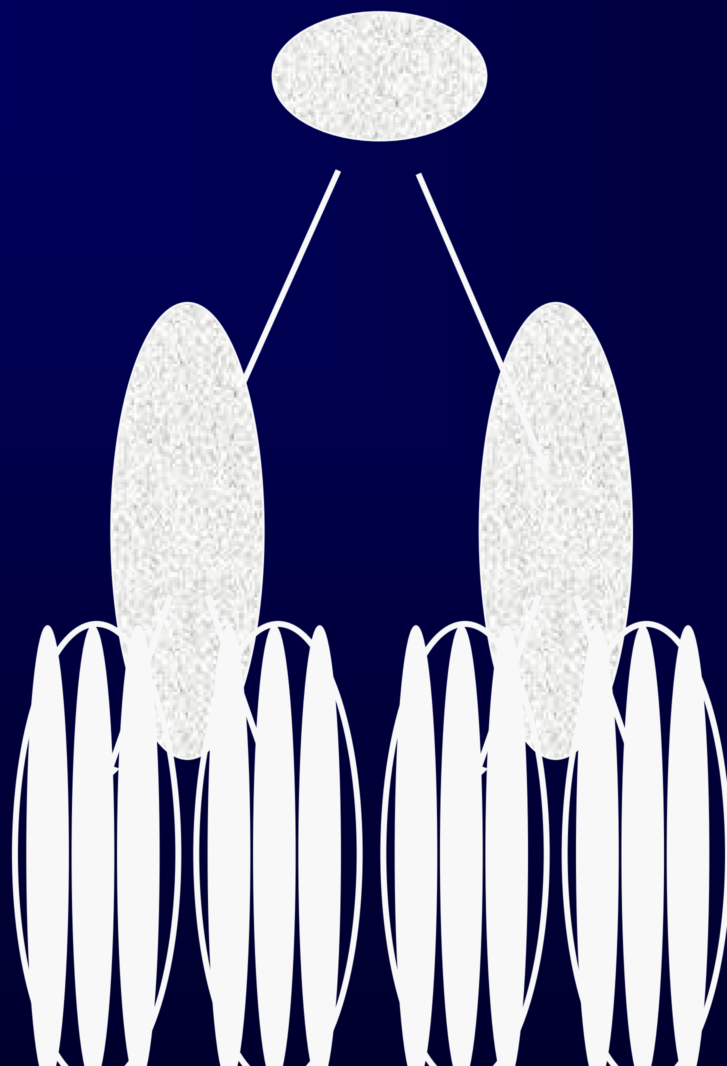
System Architecture

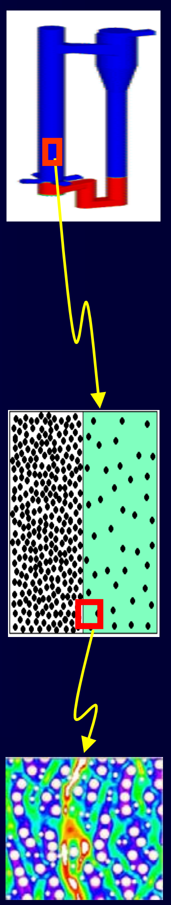
Equipment

CPU

CPU+ nGPU

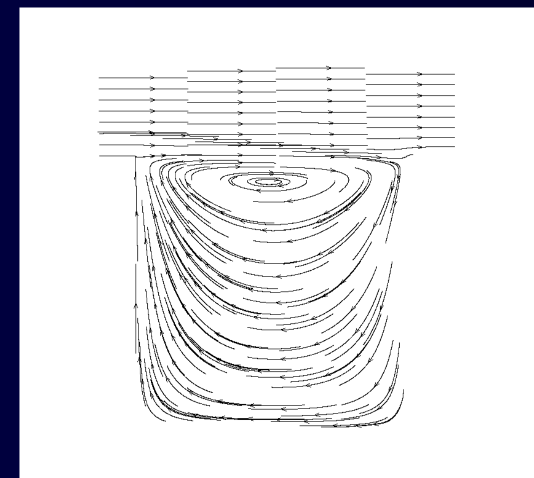
CPU+mGPU

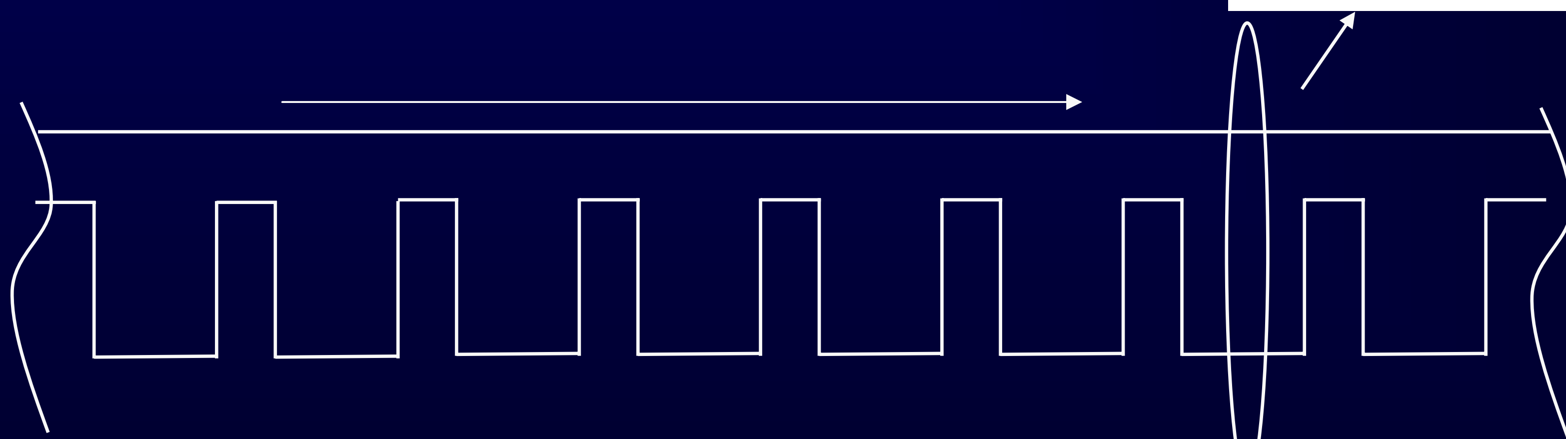




Real performance in couette-cavity flow

Mode member	Computational load	Performance (flops)	Efficiency
150T / AMD + 450T / NV	.5×	51T	8.5%
	1×	102T	17%
	2×	162T	27%
	5×	324T	54%



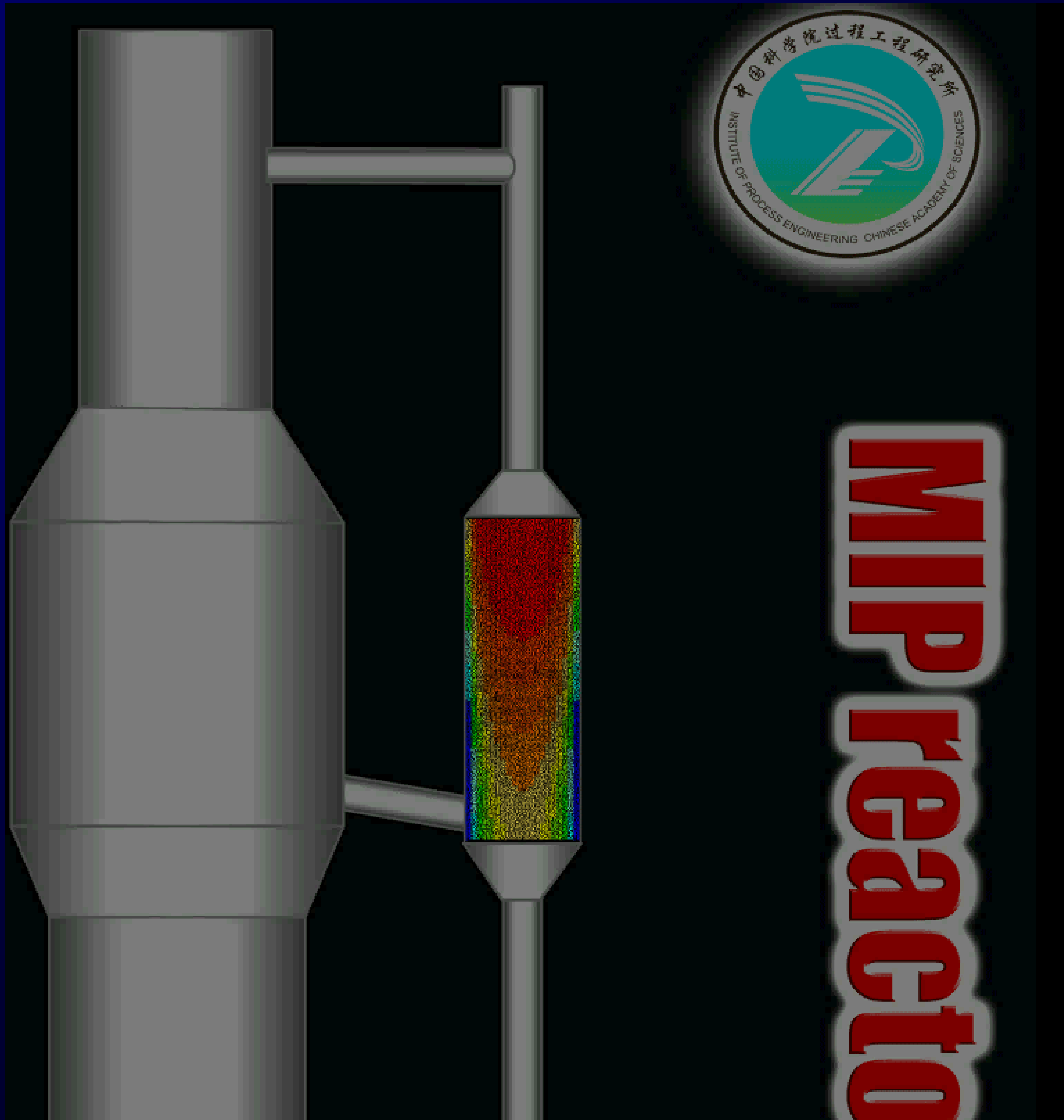


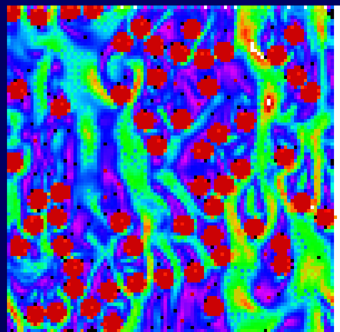
Grooved micro-channel 1024x1024x4

Simulation of gas-solid system

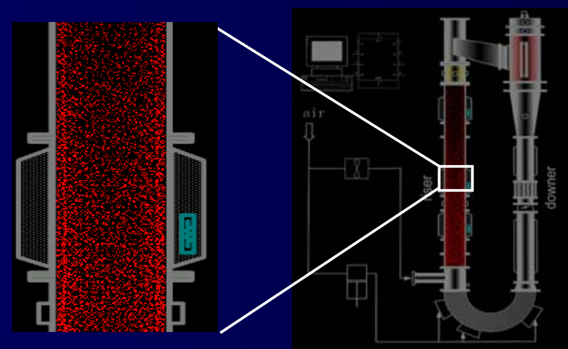
Comparison of capability

- **120T (GPU)** → **1 Day**
- **1000T**
  - **GPU** → **2 Hours**
  - **Variational multi-scale** → **2 Minutes**

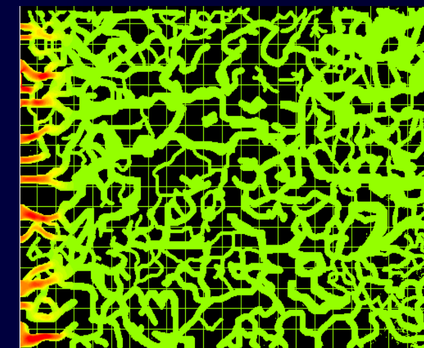

中国科学院过程工程研究所
INSTITUTE OF PROCESS ENGINEERING CHINESE ACADEMY OF SCIENCES
MIP reacto



1024 Particles

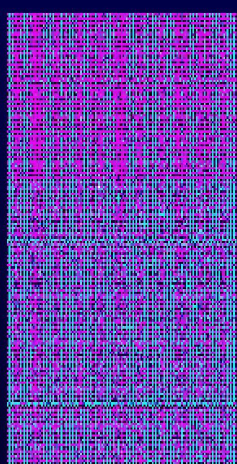


Experimental apparatus

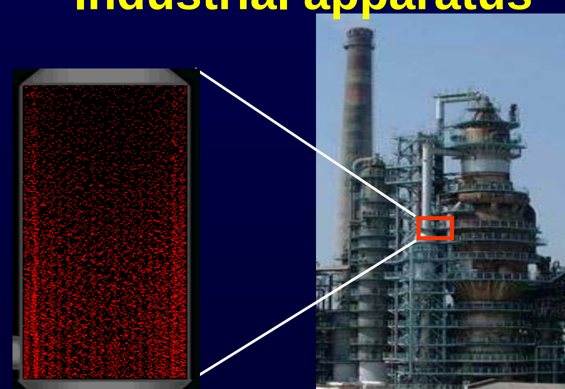


Sample of rock

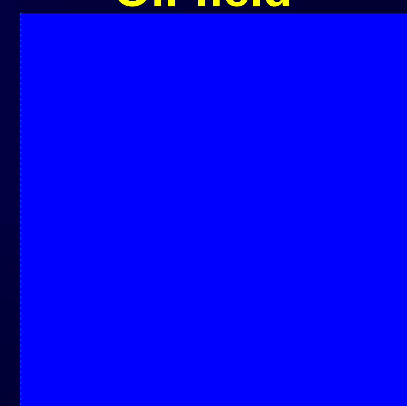
20000 Particles

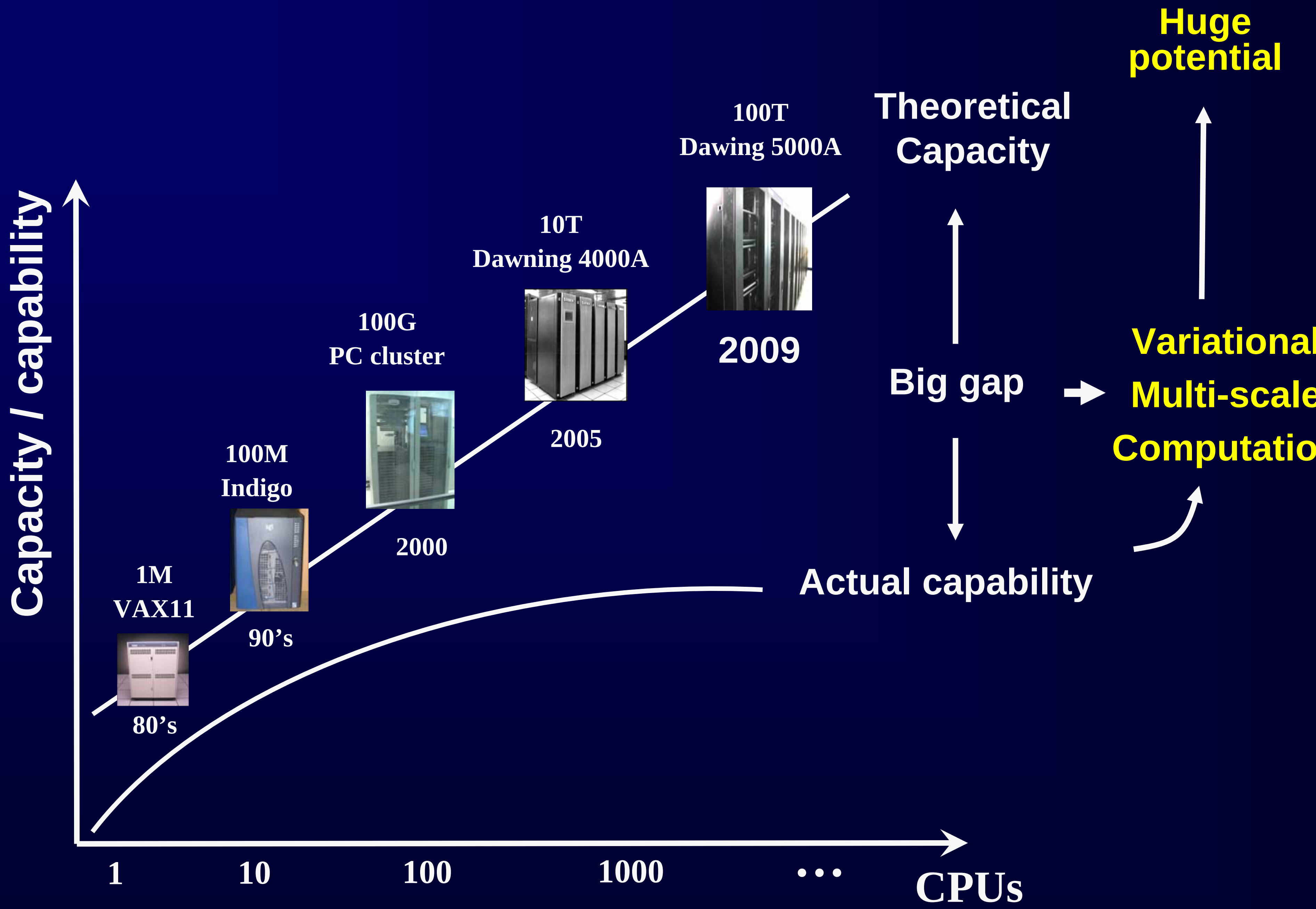


Industrial apparatus



Oil-field

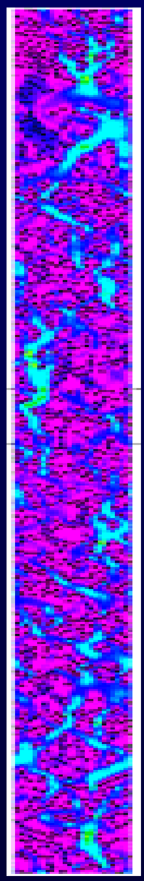



Huge
potential
100T
Dawing 5000A
Theoretical
Capacity
10T
Dawning 4000A
2009
100G
PC cluster
Variational
Multi-scale
Computatio
Big gap
100M
Indigo
2000
2005
1M
VAX11
90’s
80’s
Actual capability
Capacity / capability
1
10
100
1000
• • •
CPUs

Applications

Direct simulation of gas/solid system

2006



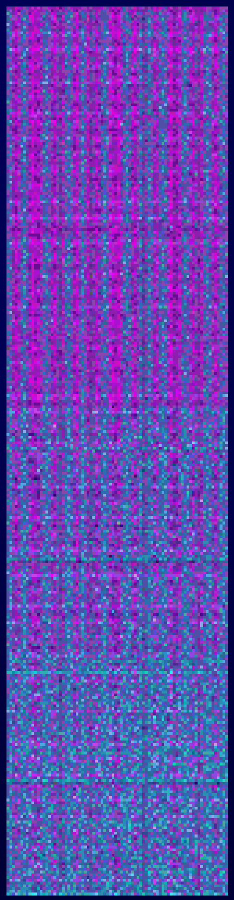
Ma et al., Chem. Eng. Sci., 61: 7096,2006.

Ma et al., Chem. Eng. Sci., 64: 43,2008.

1024 Particles

1024CPU

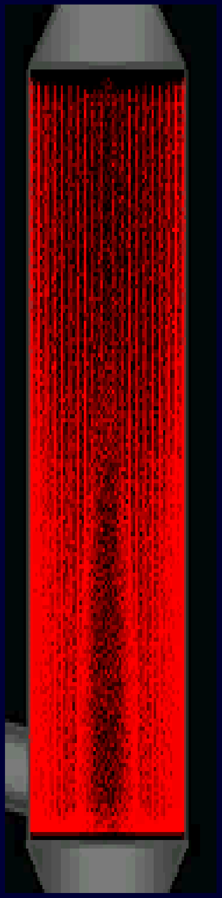
2008



25 K Particles

200GPU

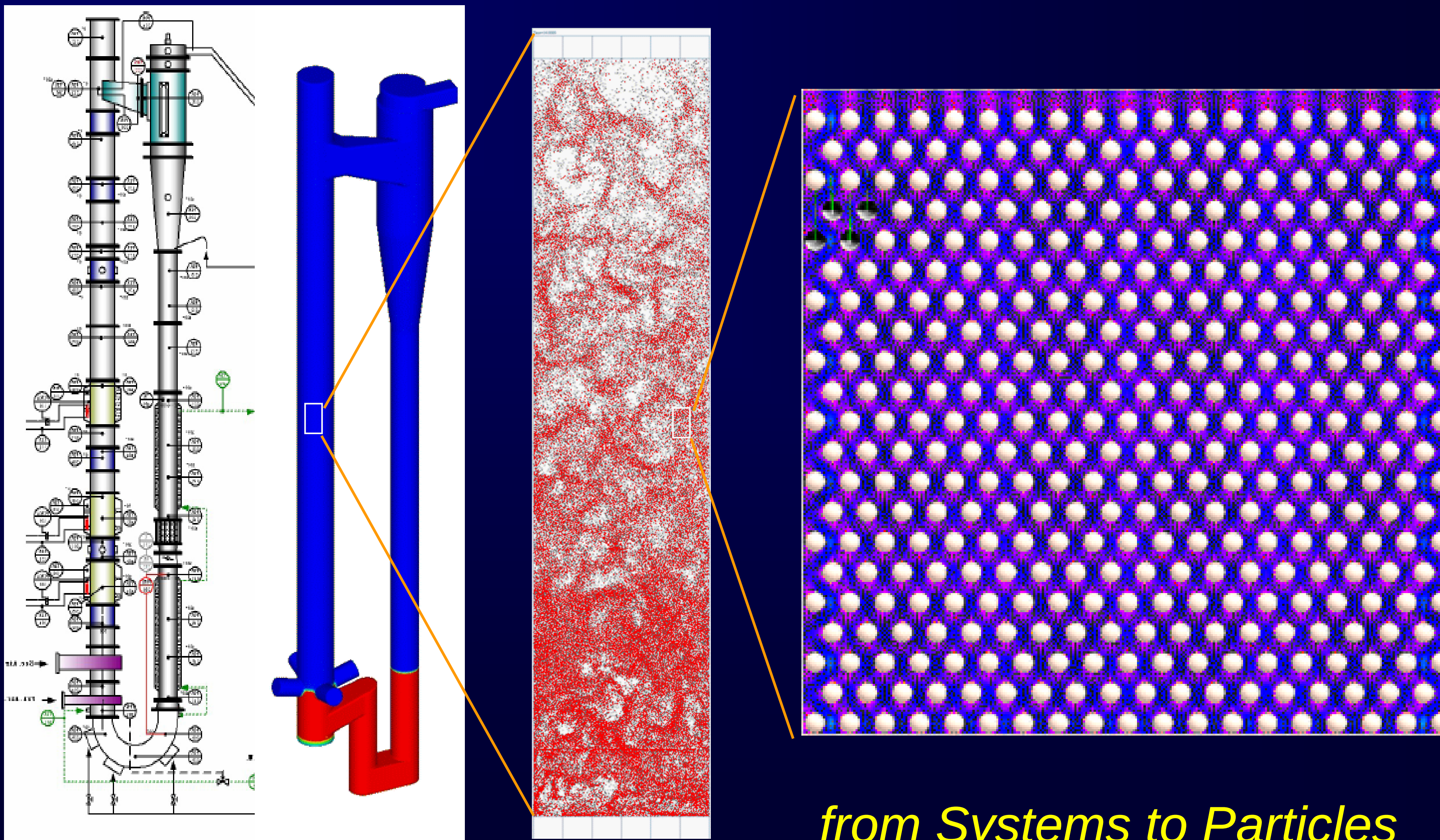
2009



2.5M Particles

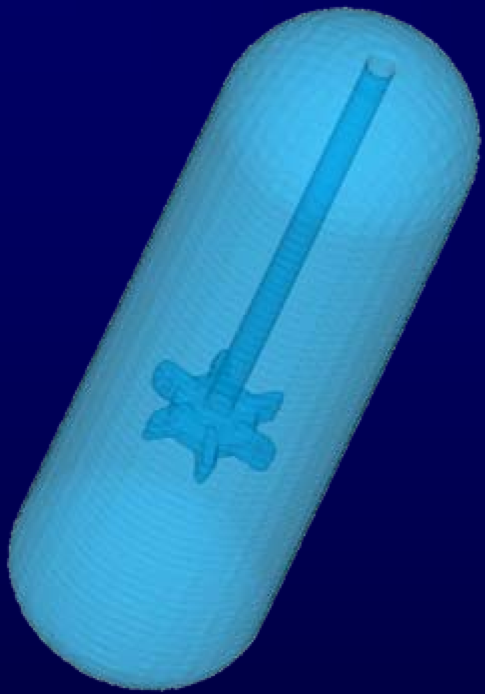
240GPU

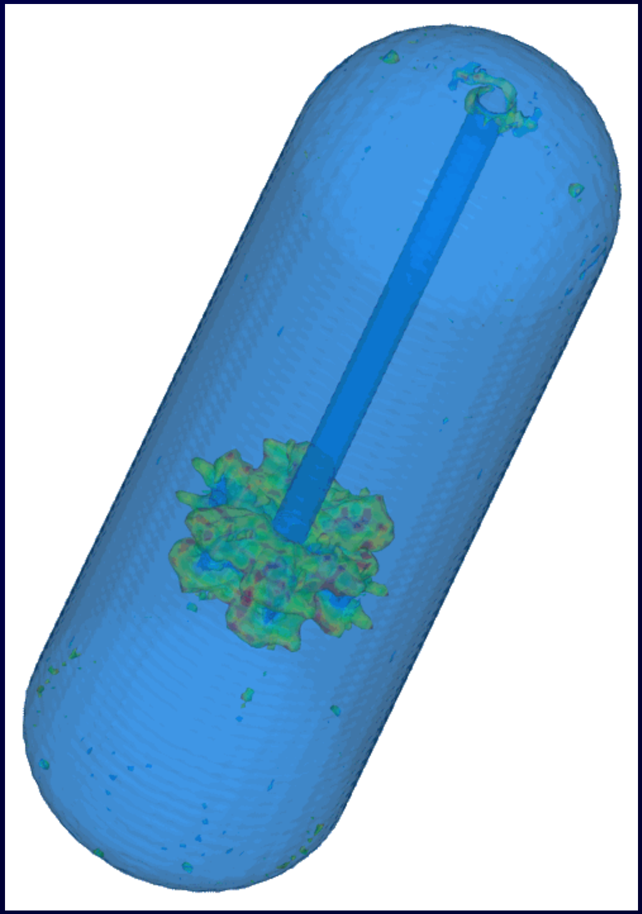
GPU computation :
100K Particles +200M pesudo-particles



from Systems to Particles

Direct simulation of industrial stirred tank





Commercial software

2D steady

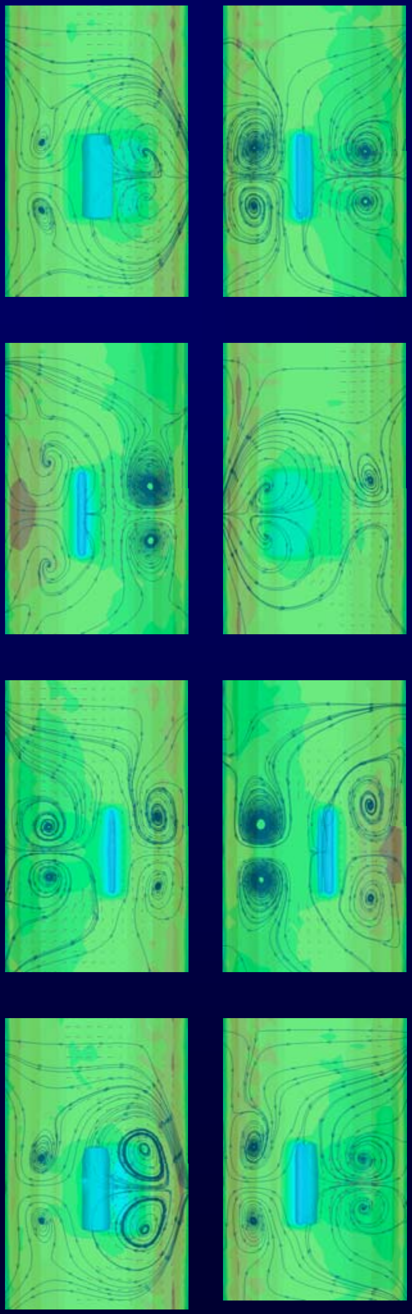
Parallel computation

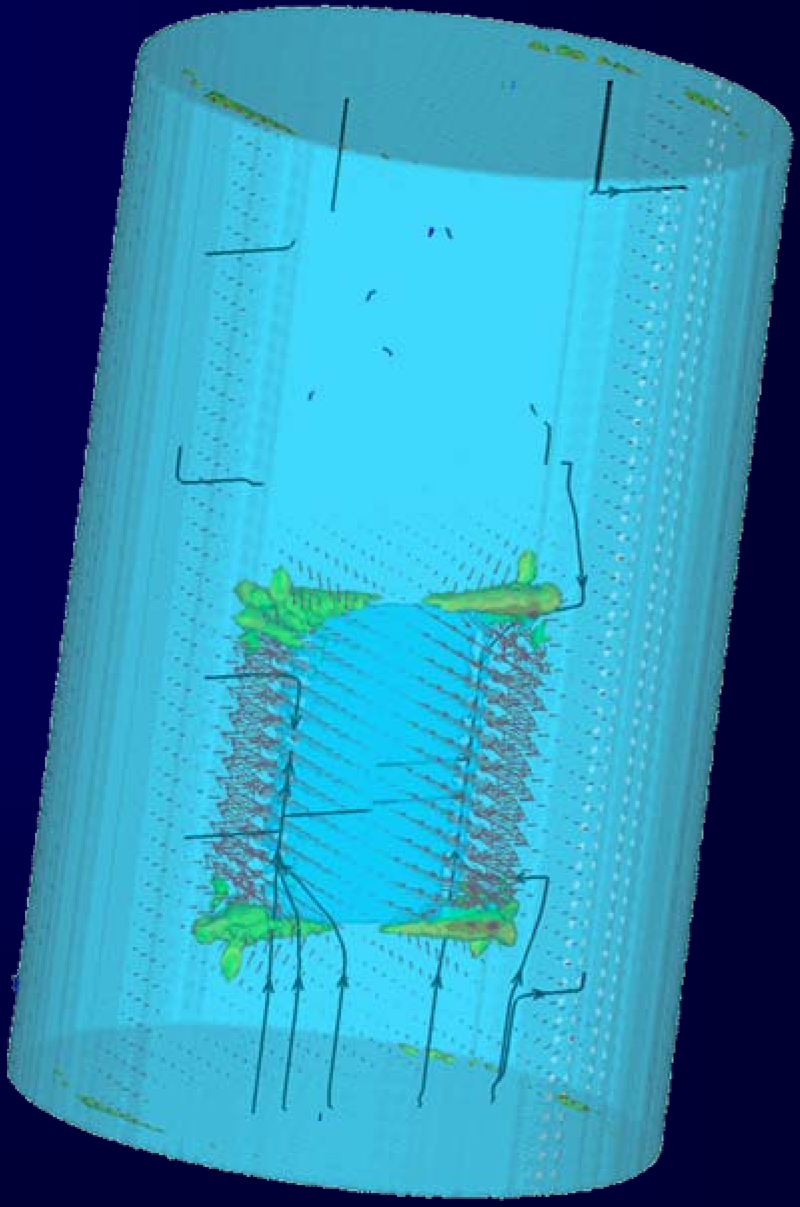
→

200GPU

This system

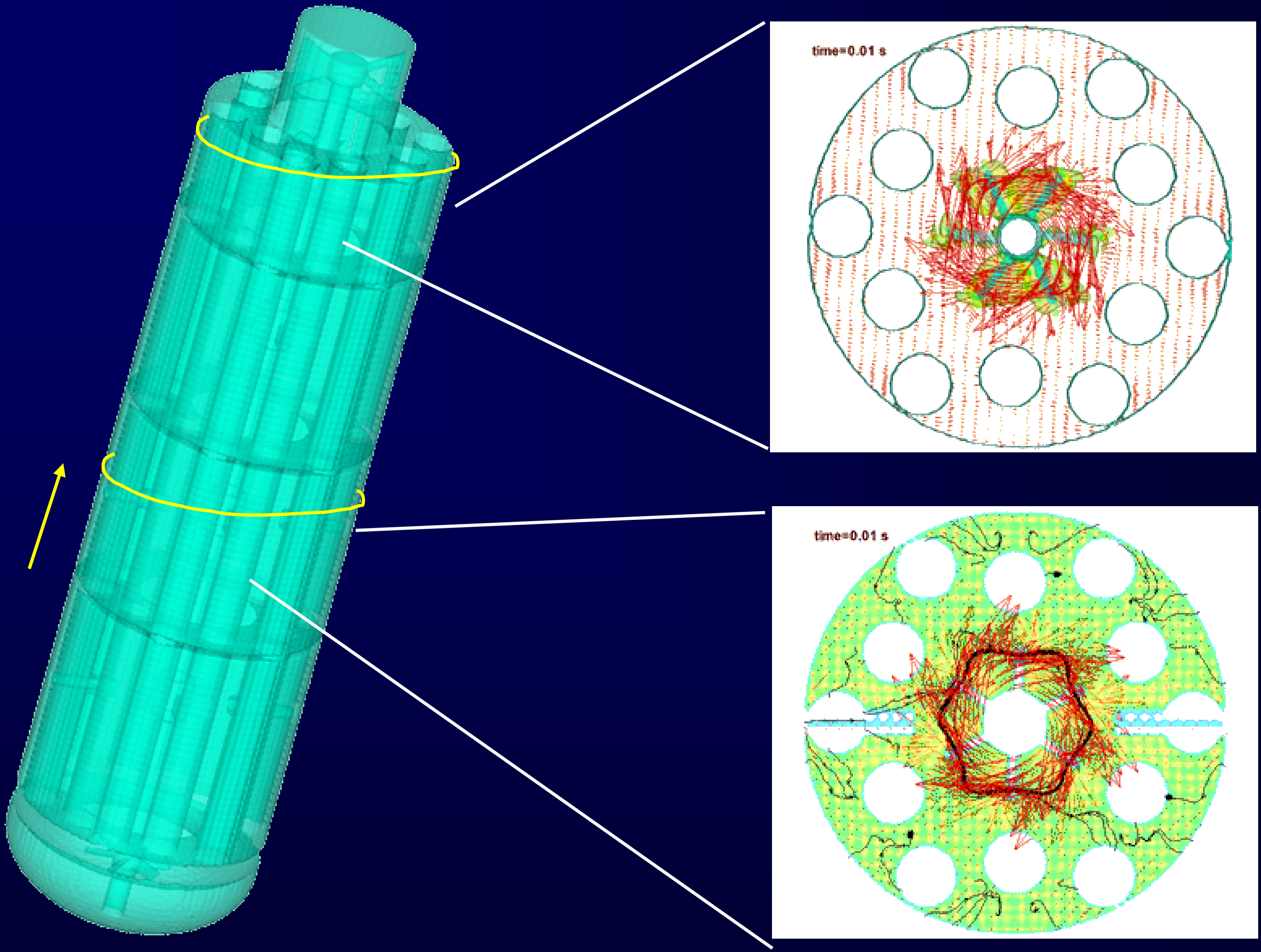
3D Dynamic





Stirred Tank

3D MaPM, 200 GPU

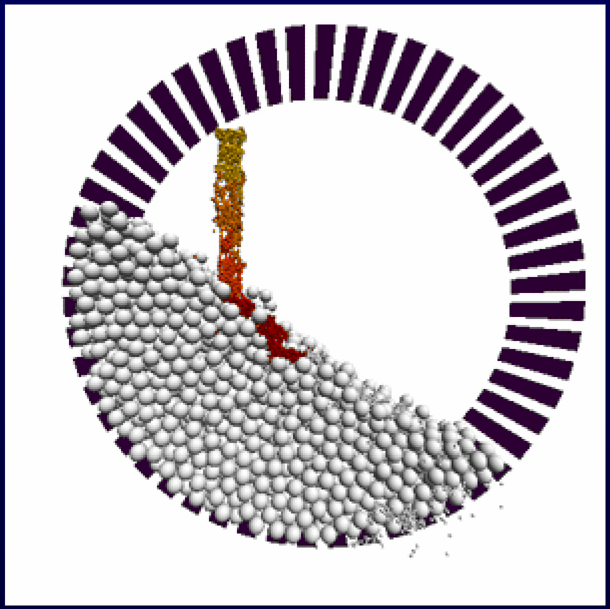


Stirred tank

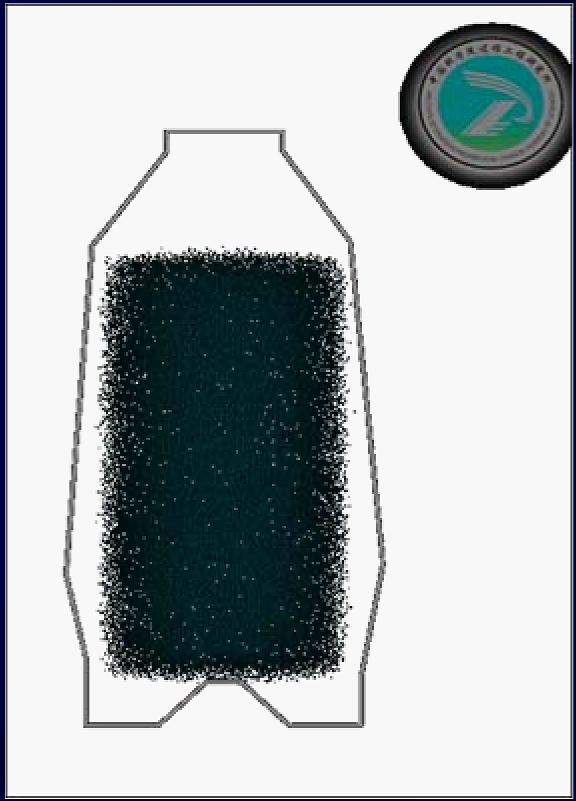
~100 M particles, 32GPU，5.5s/step，61h/round

Metallurgy process

Slurry of steel



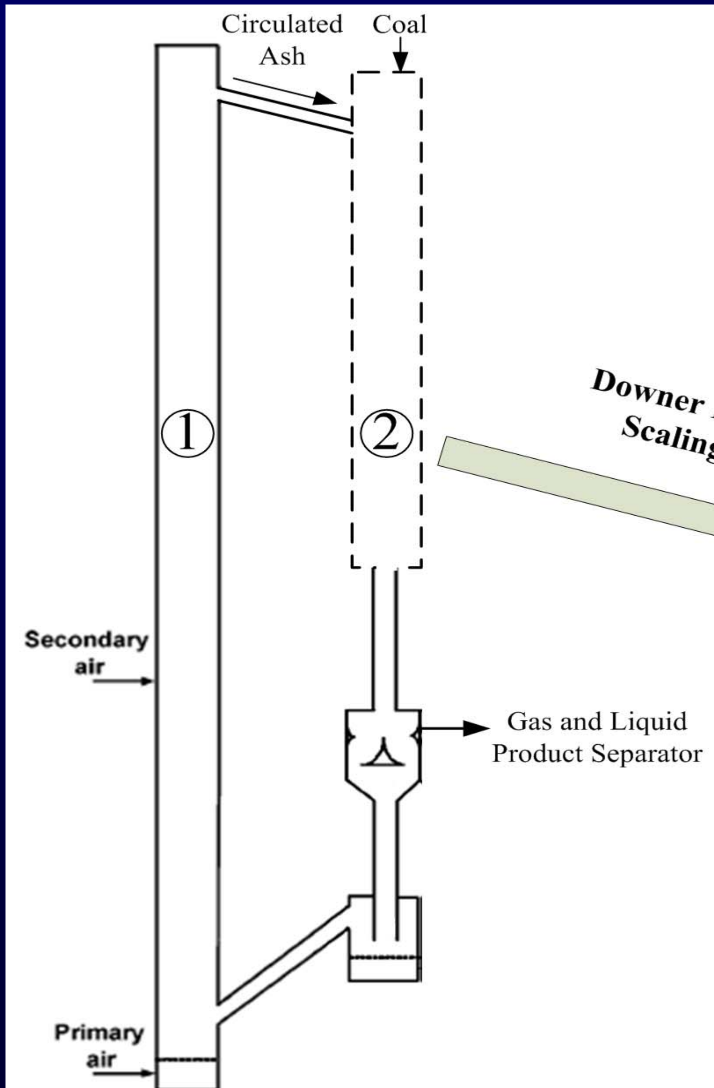
3D simulation of granular flow in blast furnace

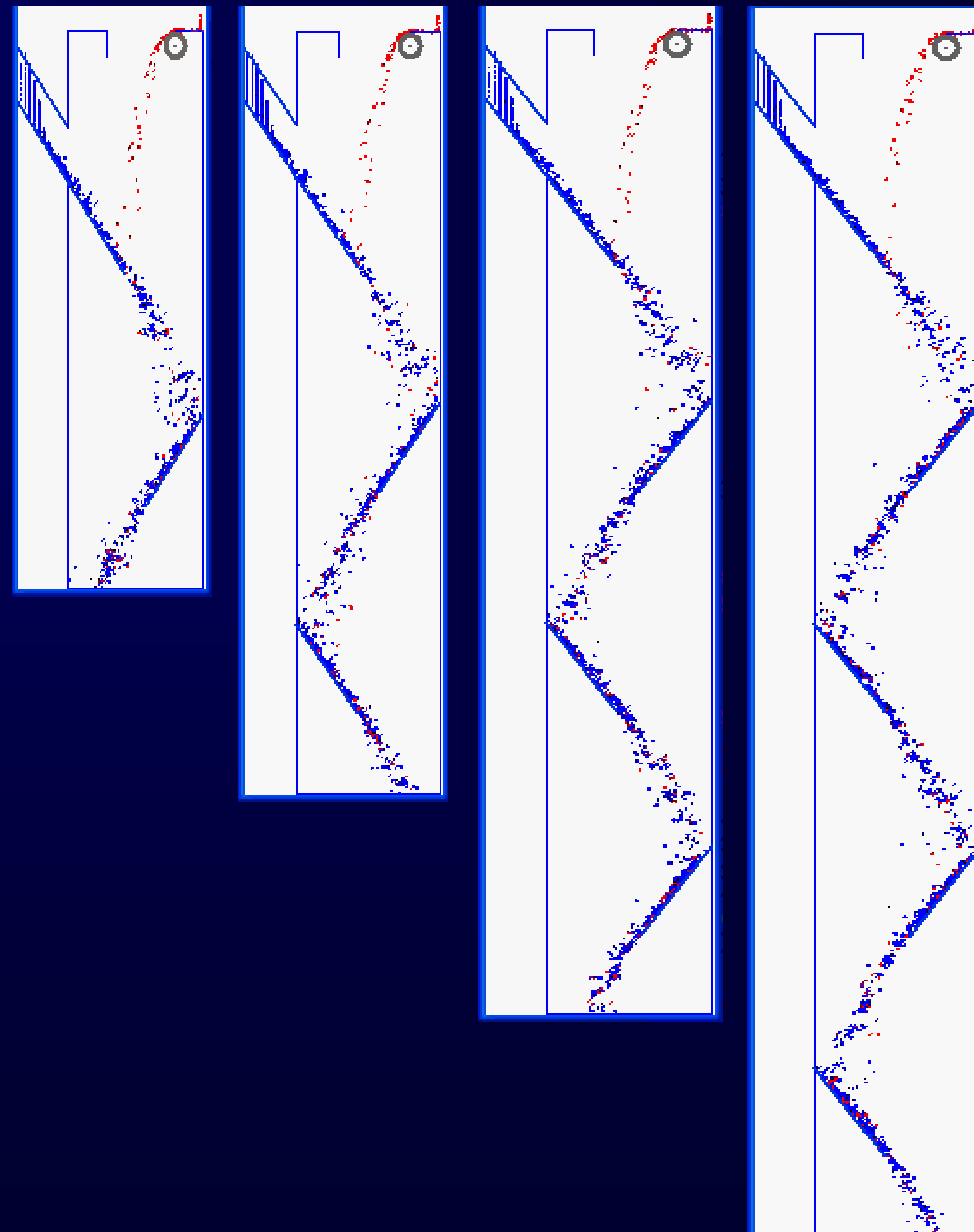


2007-08：10CPU/2GPU

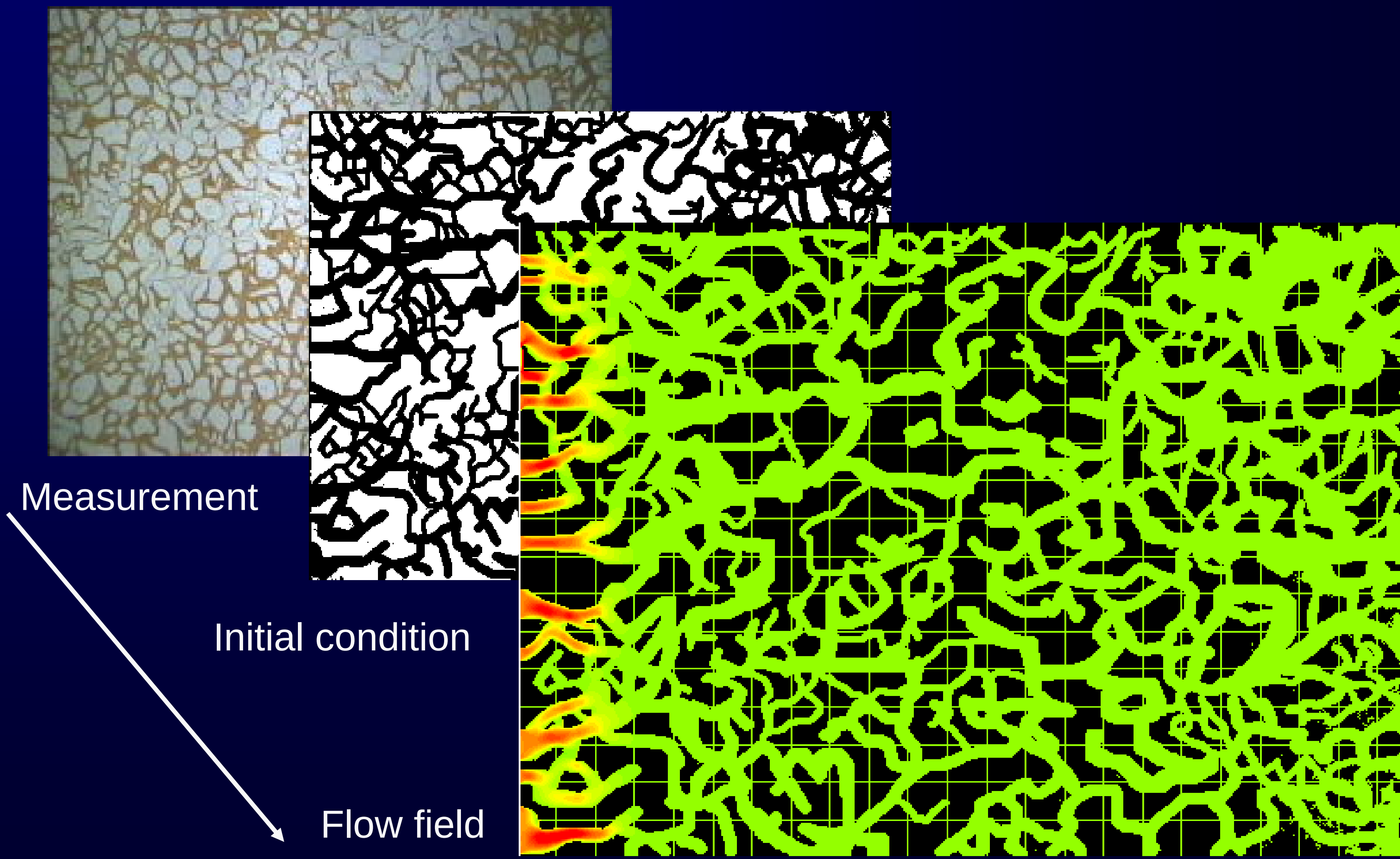
2009：20GPU

Coal-ash mixing in coal topping

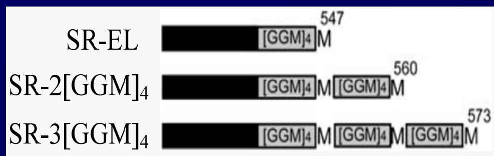


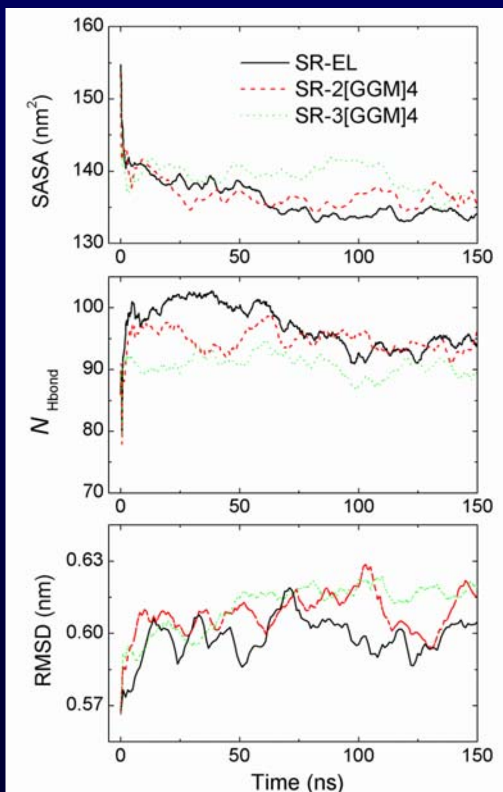


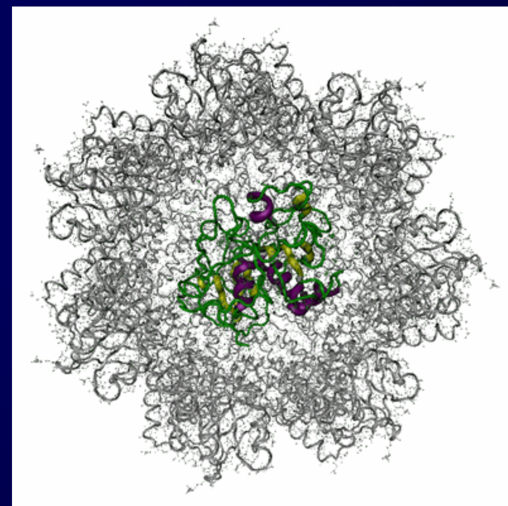
DNS of flow in porous media

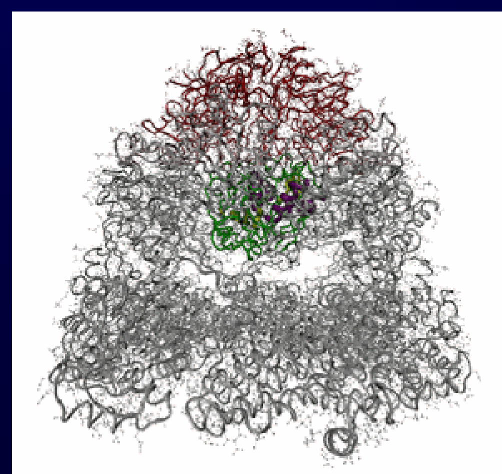


Protein folding in vivo

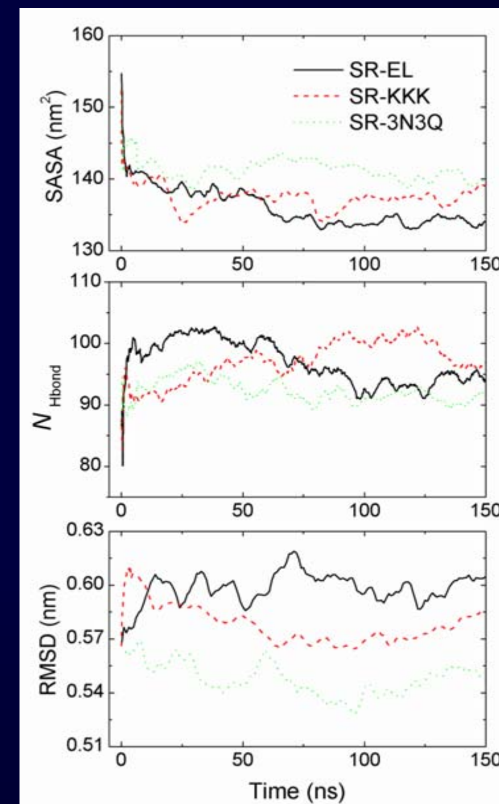




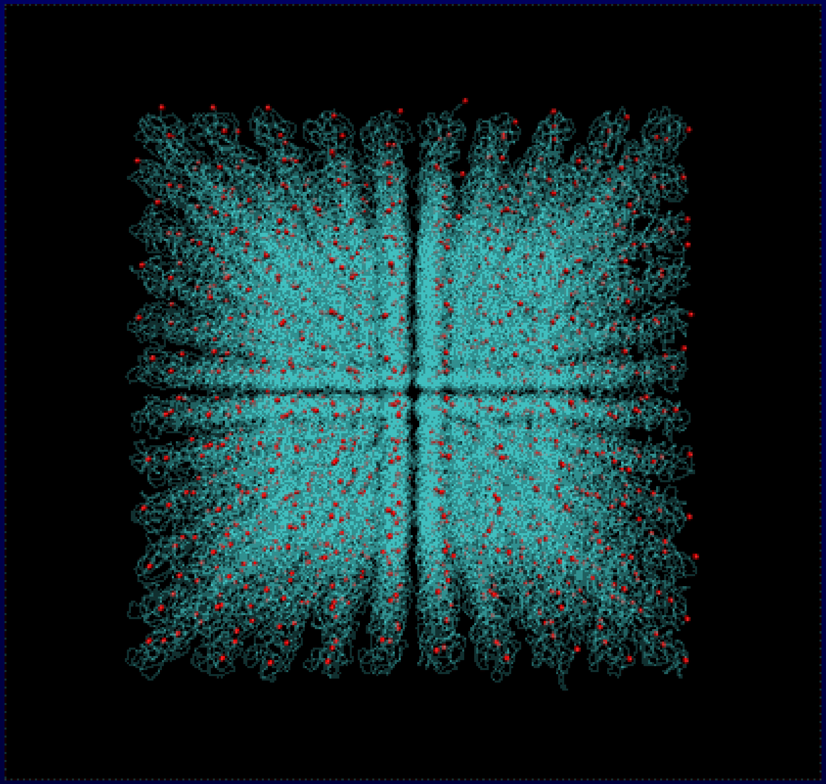




SR-KKK D358K, D360K, E362K
SR-3N3Q E251Q, D252N, E254Q, D358N, D360N, E362Q



Polymer dynamics

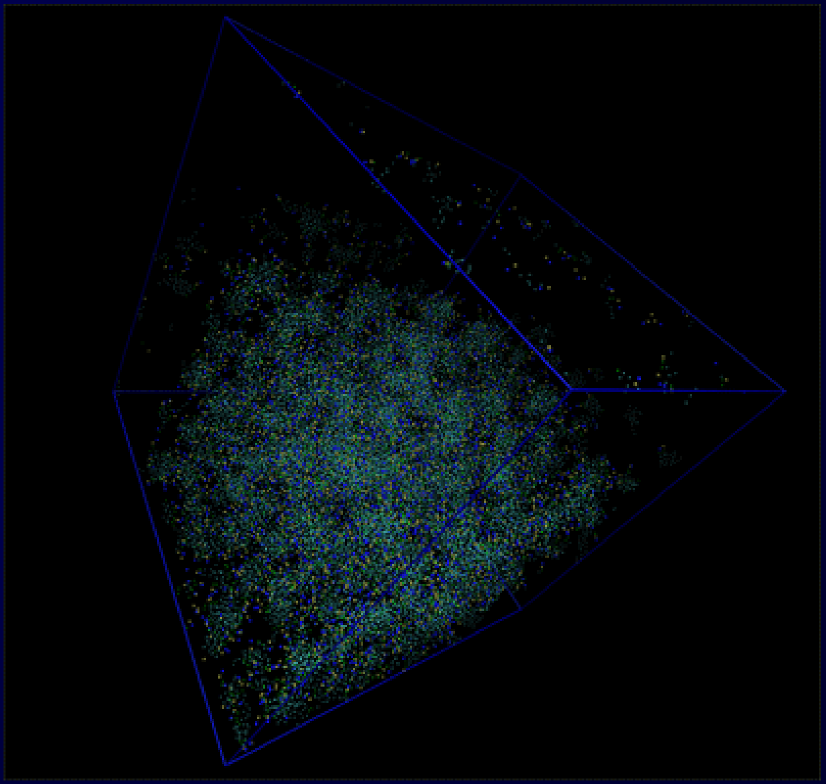


1200 polyethylene chains

Chain length：300 CH_2

NVT Ensemble

Vesicle formation



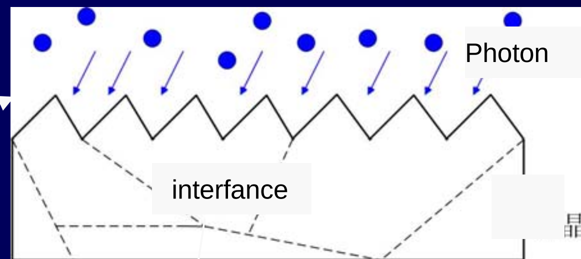
1392656 water

3375 dipalmiteyl phosphatidyl choline

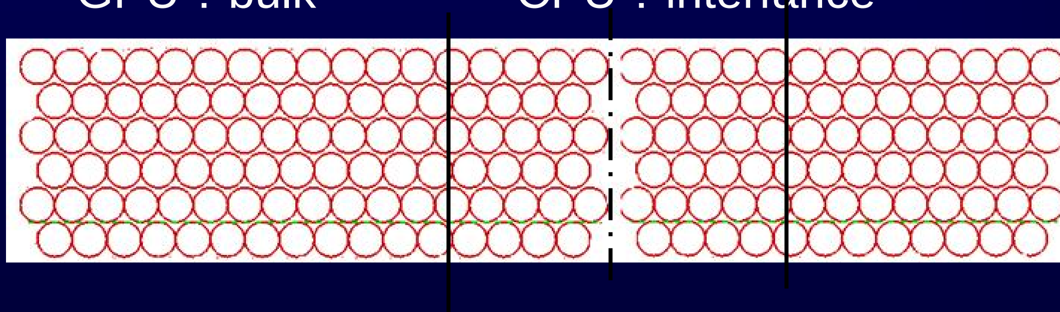
NPT Ensemble

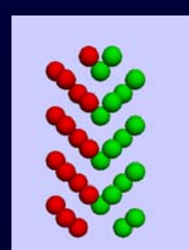
Silicon crystal for solar cell

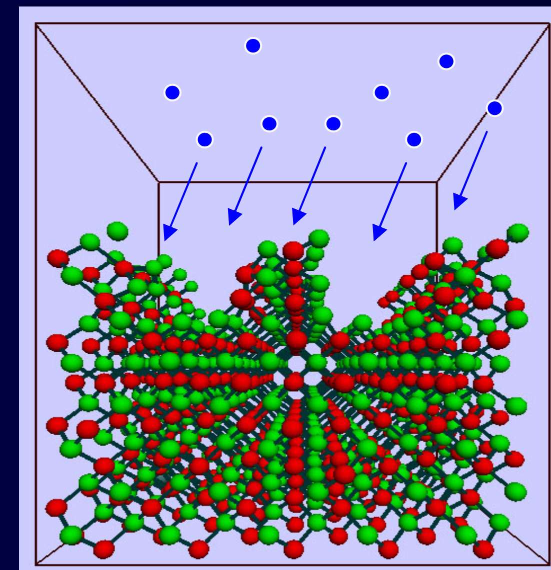
Solar cell



GPU : bulk CPU : interfance







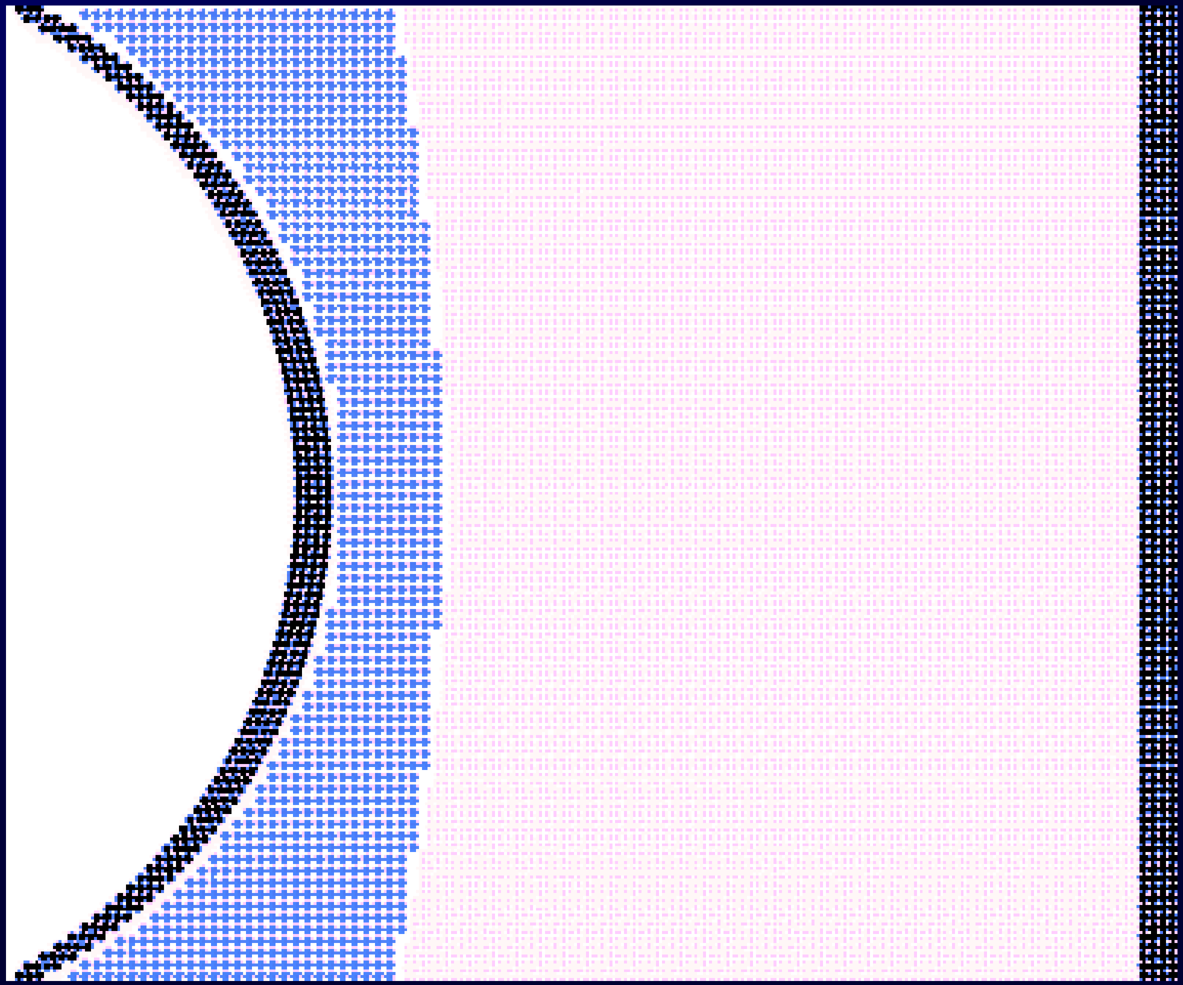
Atom number : 10^{10}
Scale : $1\mu m^3$ → Thickness on silicon film

From Angstroms to Microns:

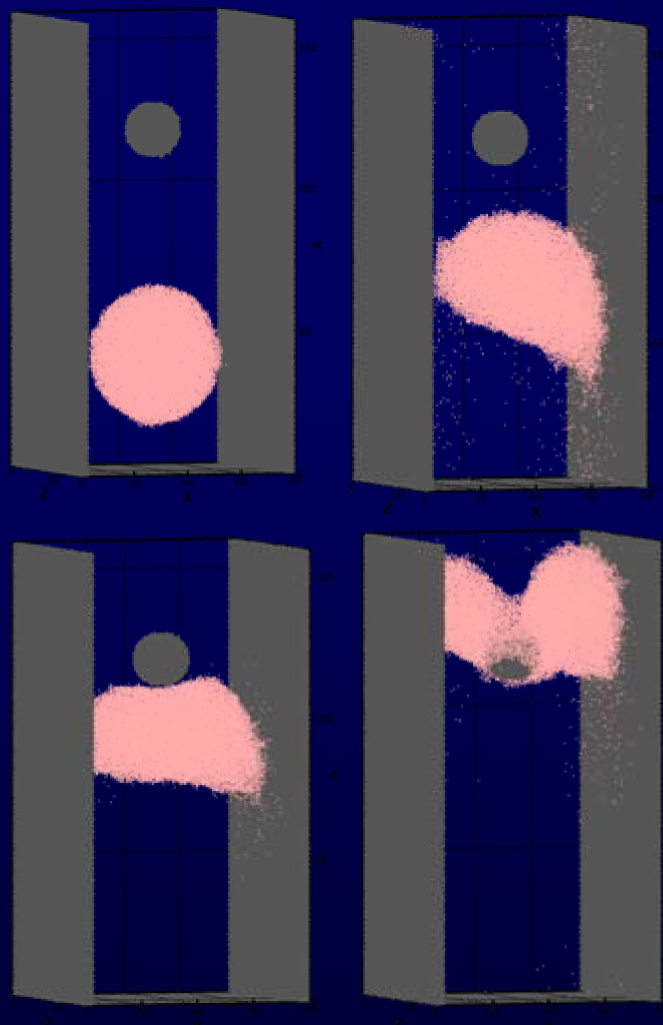
MD-PPM simulation of interactions

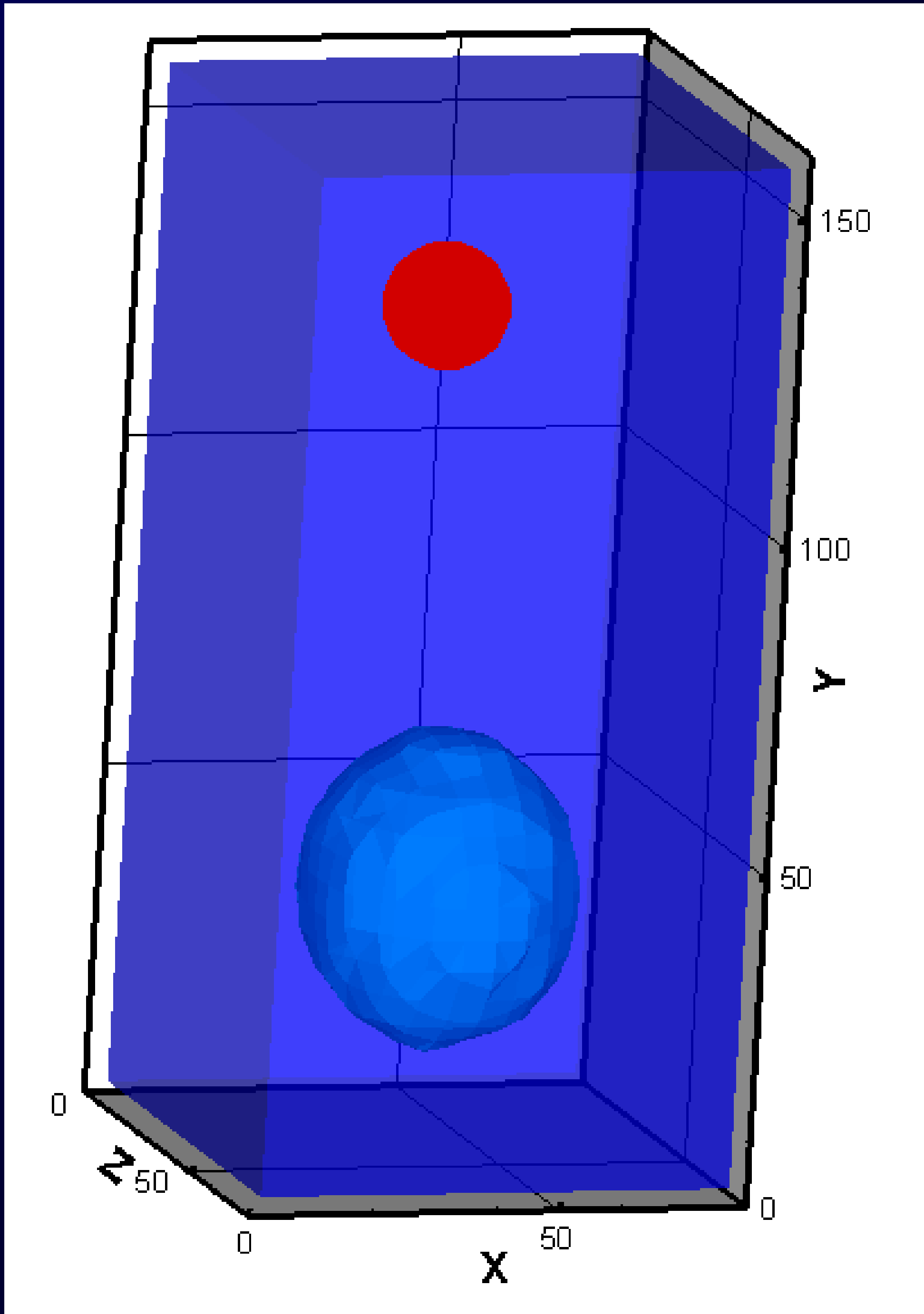
2D simulation of
liquid film rupture
40nm×35nm,
solid velocity 3.2m/s
LJ/PP fluid at 60K,
constant P & V

10000 particles,
3.2G Intel CPU
(1core)



Chen et al., Sci. in China,52,2008,372-380





3D simulation: bubble-particle in liquid

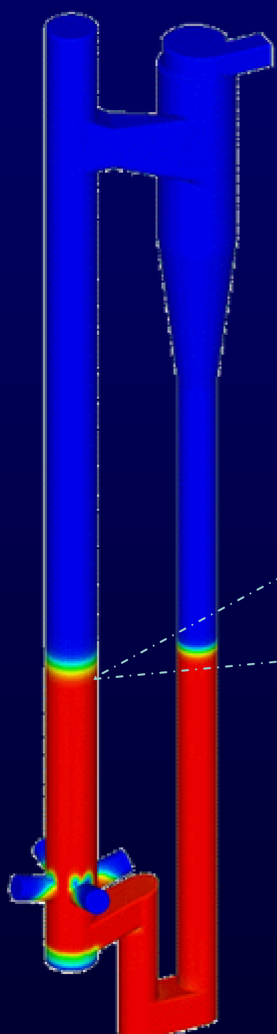
0.1*0.1*0.15μm, bubble mean velocity 3m/s

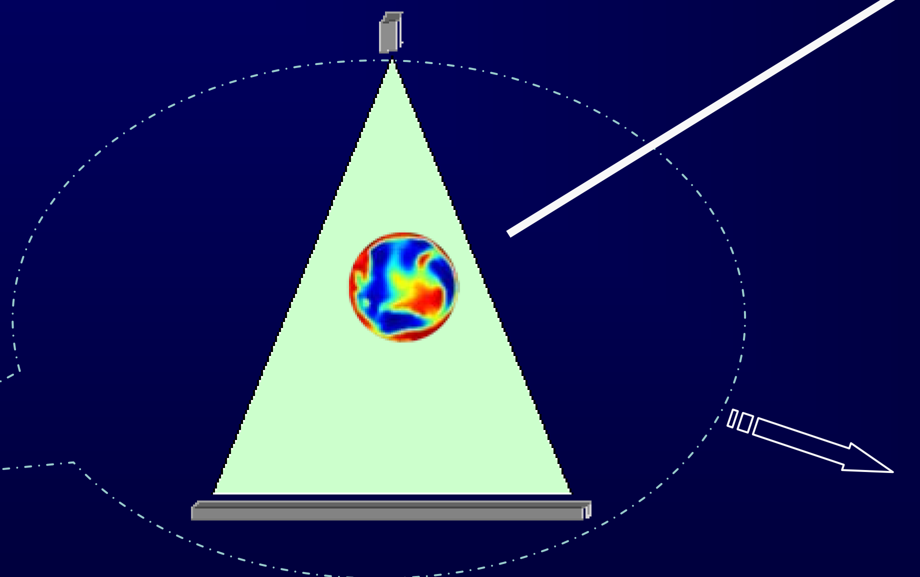
LJ/PP fluid at 60K, NVT ensemble

7M particles, 2 GPUs

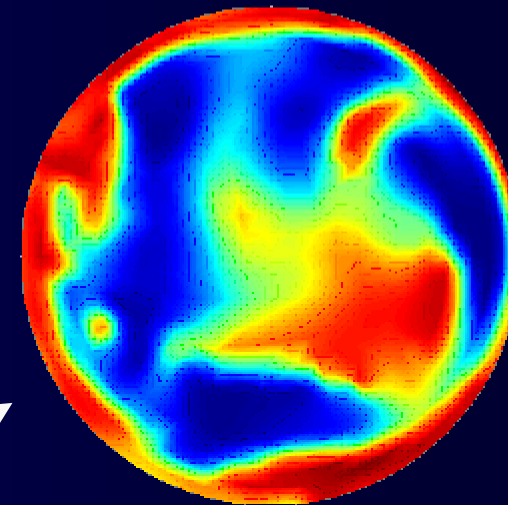
Real-time CT

Image Reconstruction

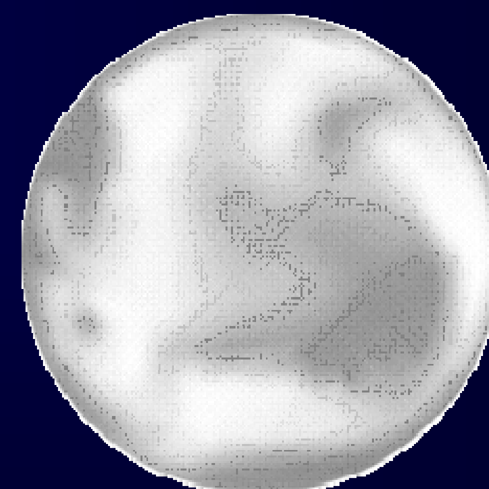




CT Scanister



On-line



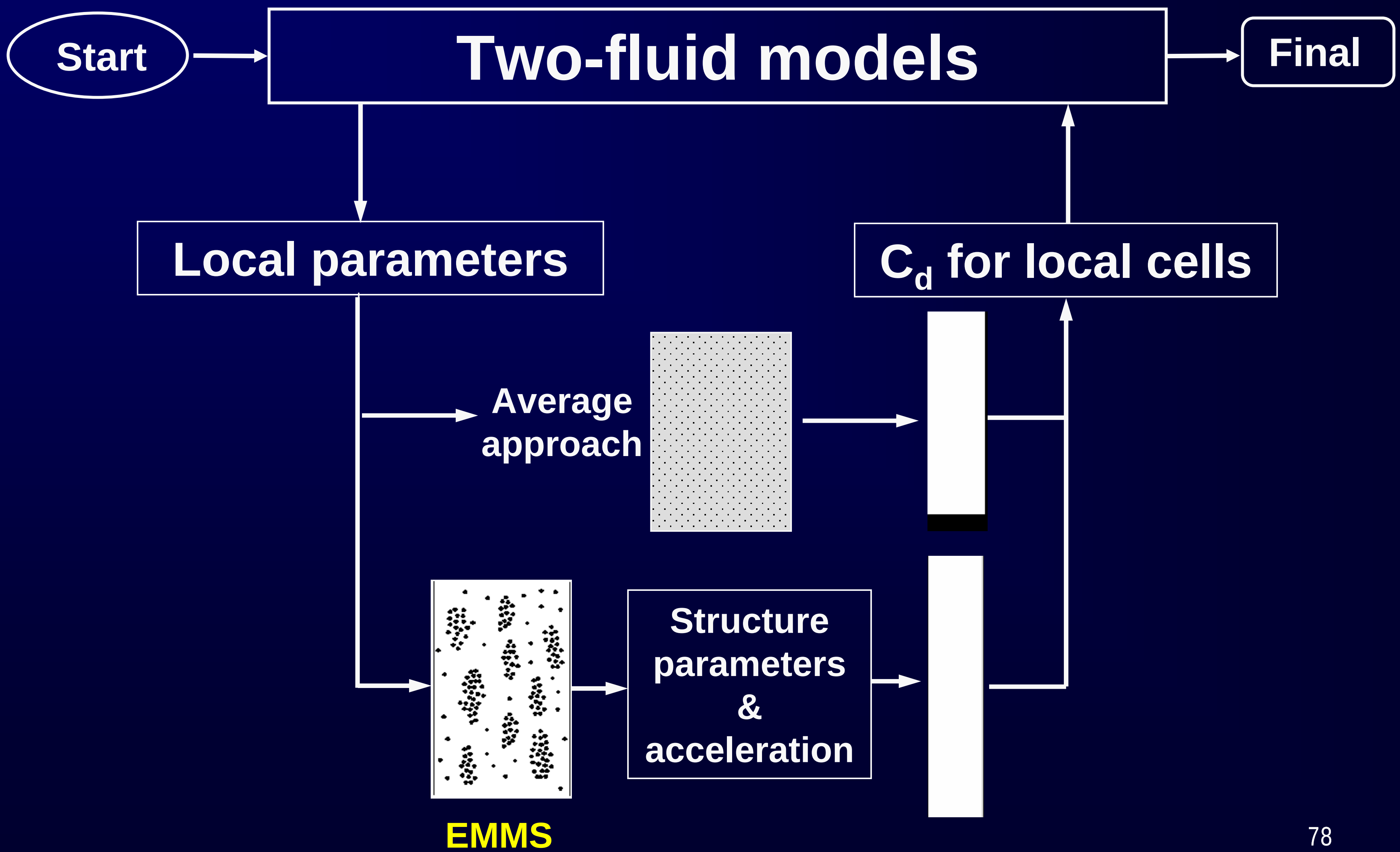
Off-line

CFD+EMMS

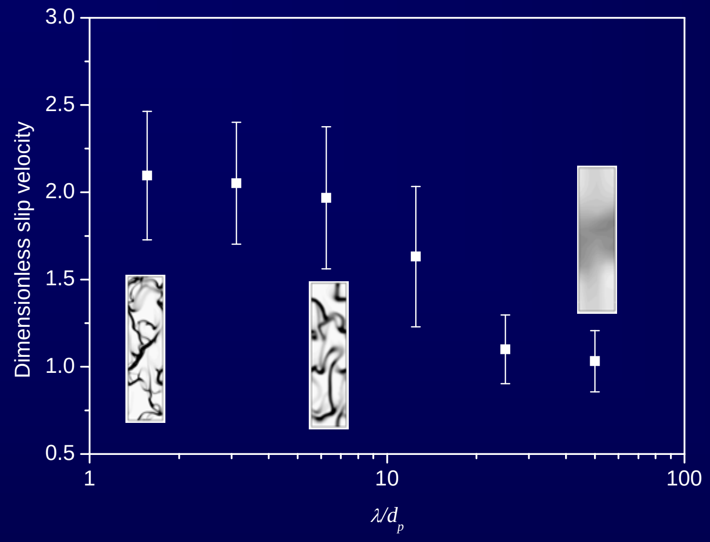
Two-fluid model

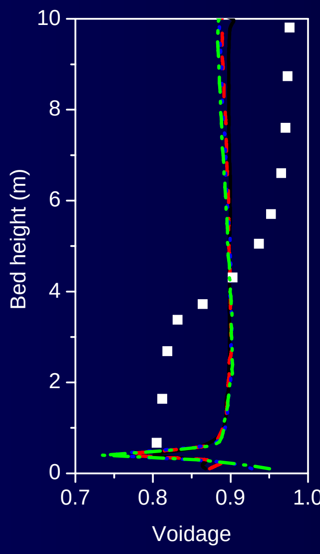
- **Limitation**
  - **Average in grid**
  - **Constitutive model**
- **Options**
  - **Smaller grid size**
  - **Meso-structure**
    - **Correlation**
    - **Stability**

Spatial-temporal correlation

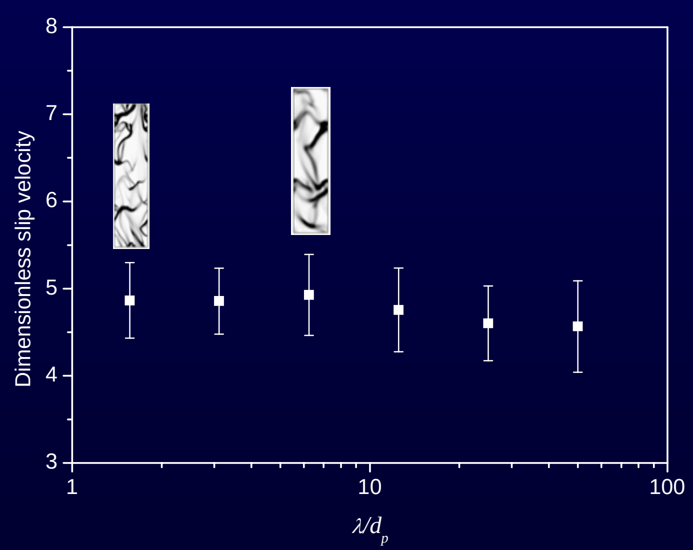


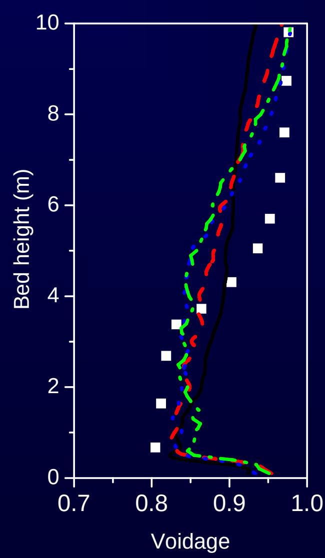
CFD + EMMS





Fine-grid TEM, big deviation from experiments

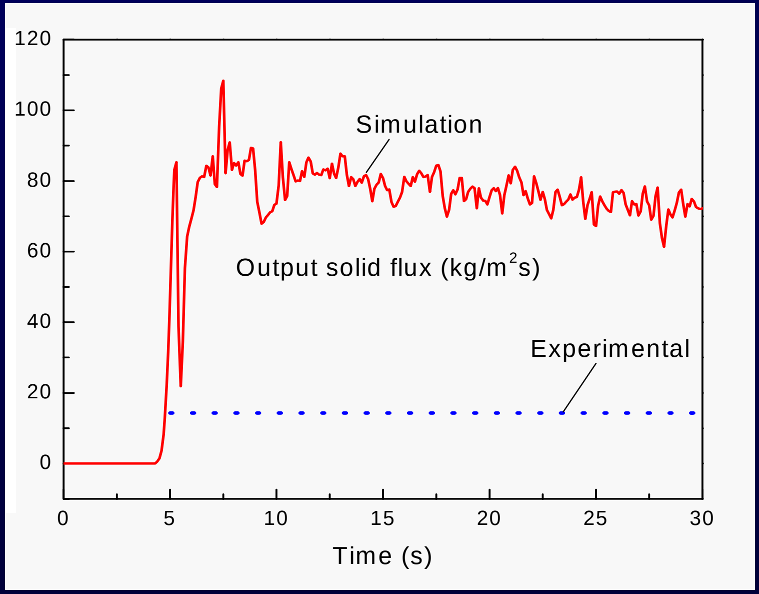




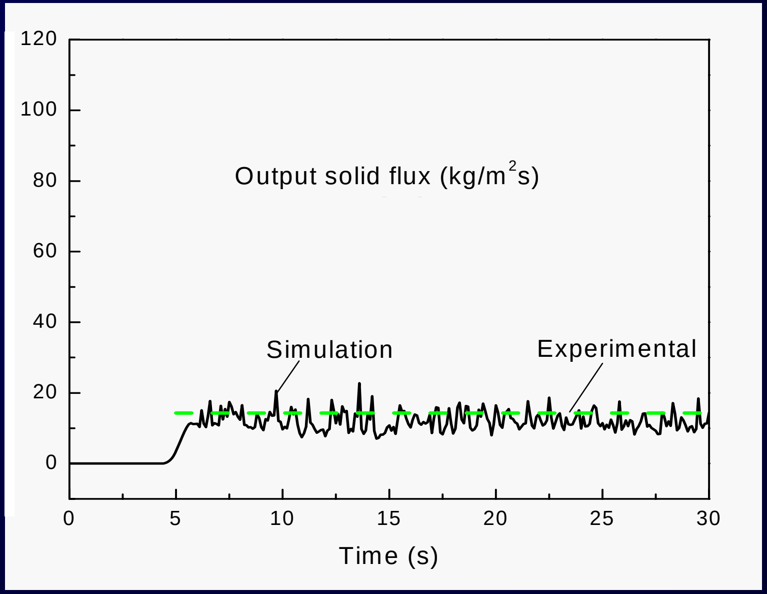
EMMS+CFD, good agreement and mesh independent

Solid flux: comparison between experiment & simulation

Simulation:
with only CFX

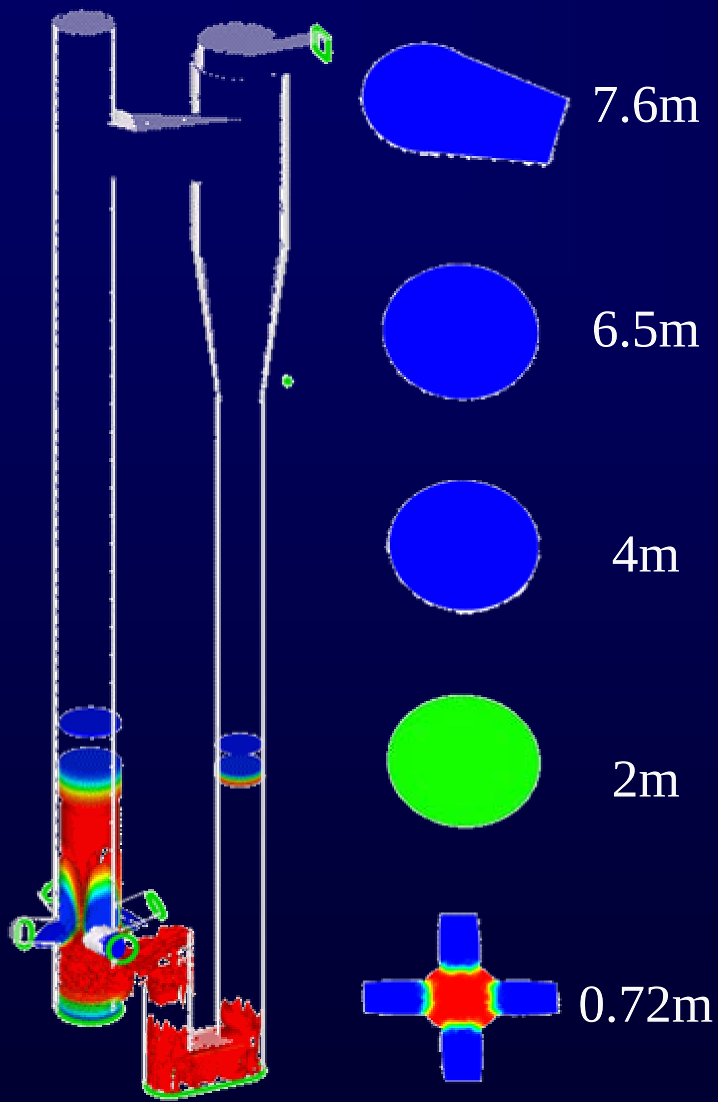


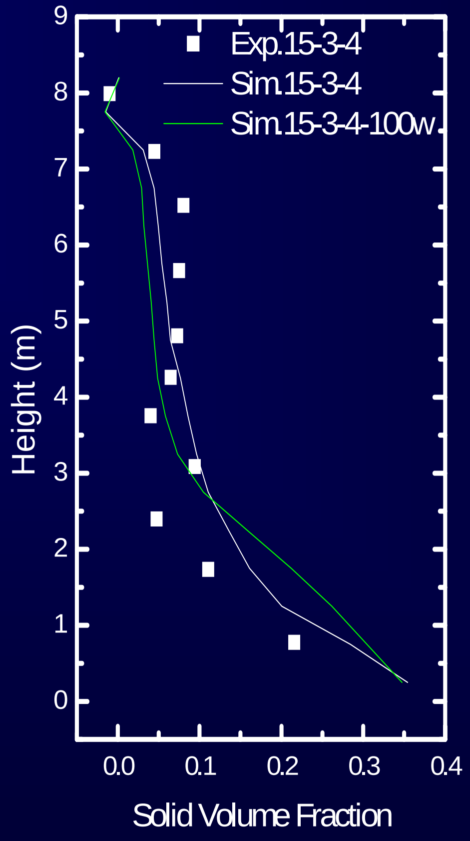
Simulation:
CFX + EMMS

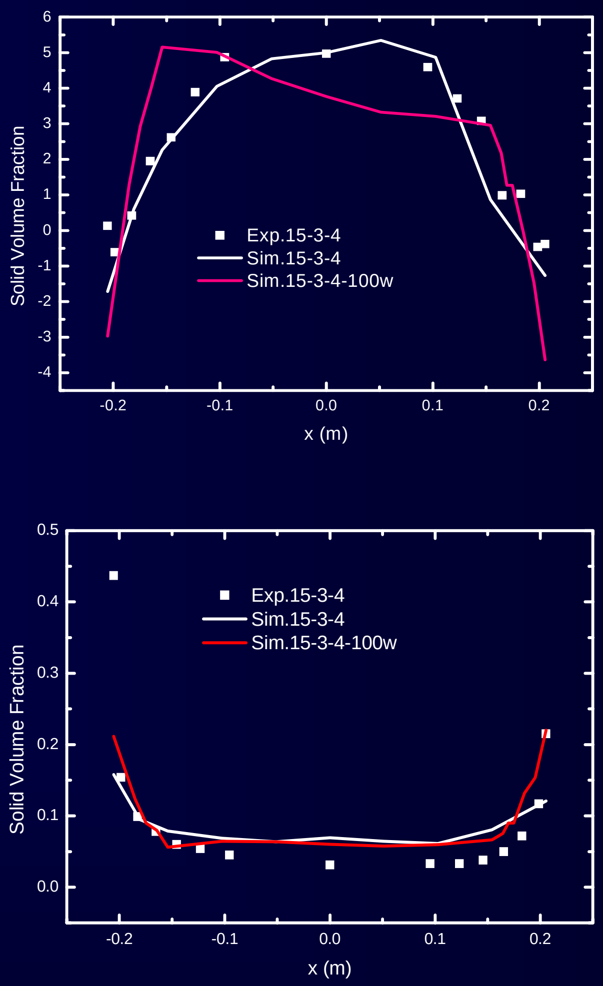


Yang, Wang, Ge & Li, Chem. Eng. J., 2003

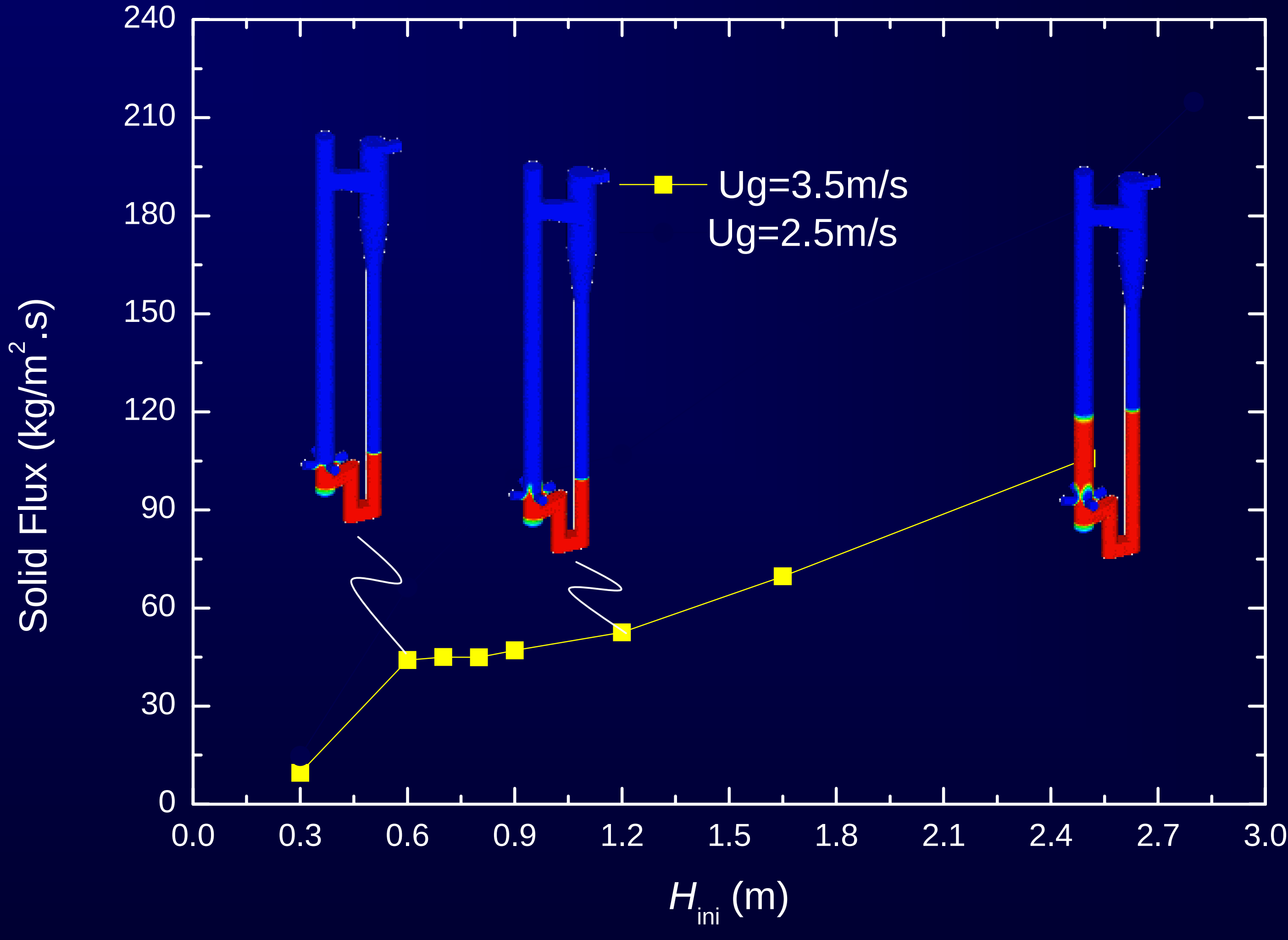
Comparison between experiment & simulation





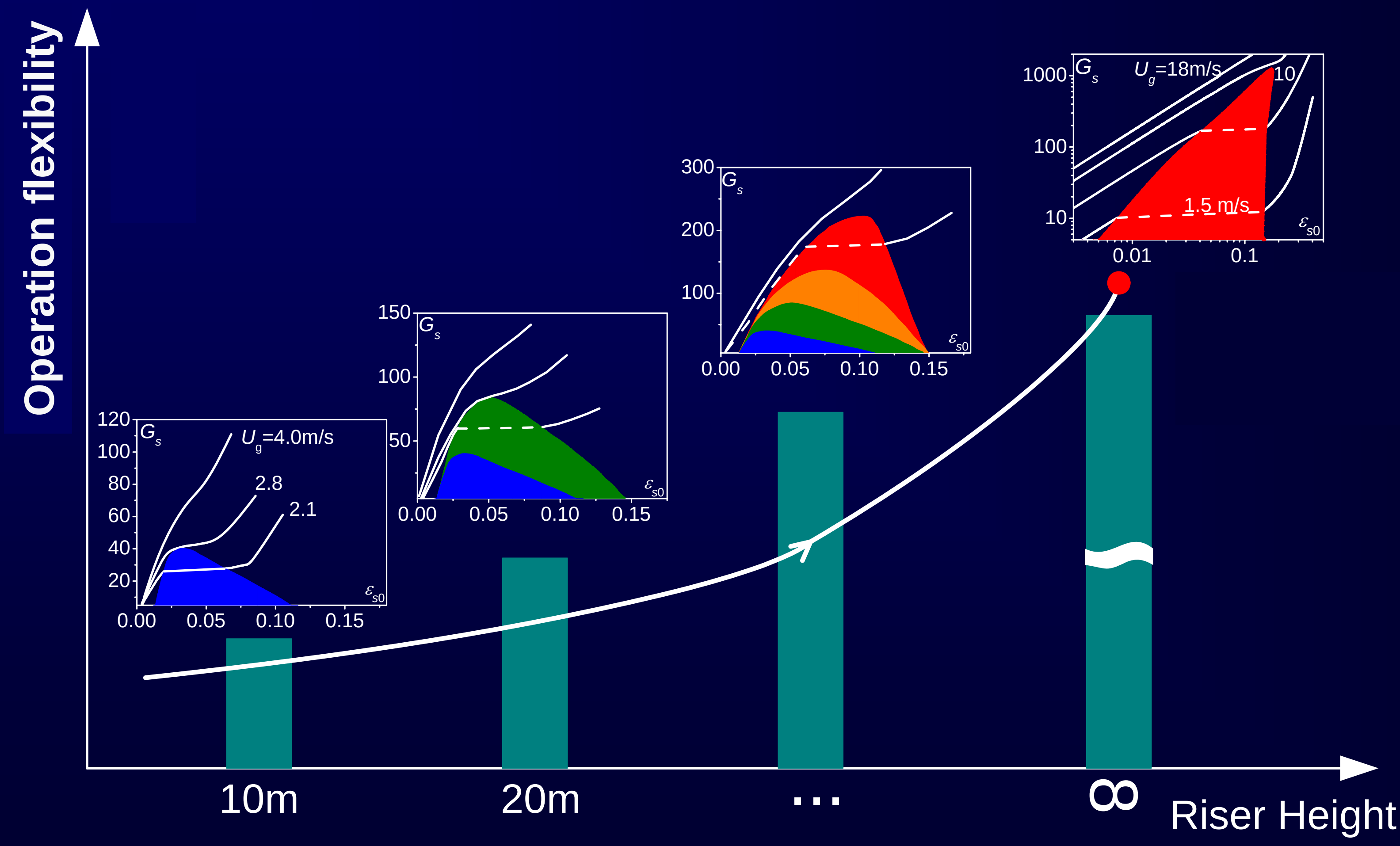


U_g = 3.5 m/s H_{init} = 1.70m



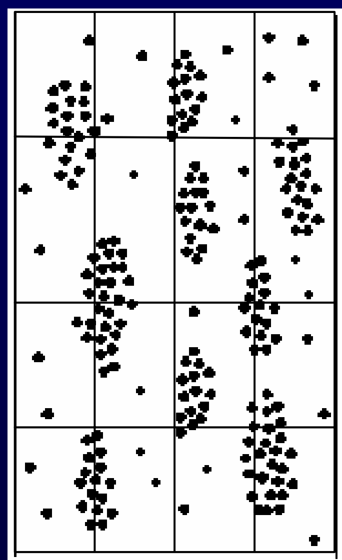
240
210
180
150
120
90
60
30
0
Solid Flux (kg/m2.s)
0.0
0.3
0.6
0.9
1.2
1.5
1.8
2.1
2.4
2.7
3.0
Hini (m)
Ug=3.5m/s
Ug=2.5m/s

Riser height is a key factor !

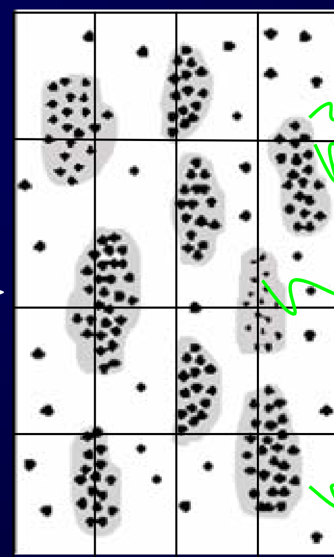


EMMS/mass: Sub-grid mass transfer

Multiscale flow



Multiscale mass transfer



$\left(\varepsilon_{gc}, \varepsilon_{gf}, f, d_{cl}, \mathbf{u}_{gc}, \mathbf{u}_{gf}, \right)$

$\left(\mathbf{u}_{sc}, \mathbf{u}_{sf}, a_c, a_f, a_i \right)$

Sh_{static}

$Sh_{dynamic}$

Meso-scale

Sh_{dense}

Sh_{dilute}

Micro-scale

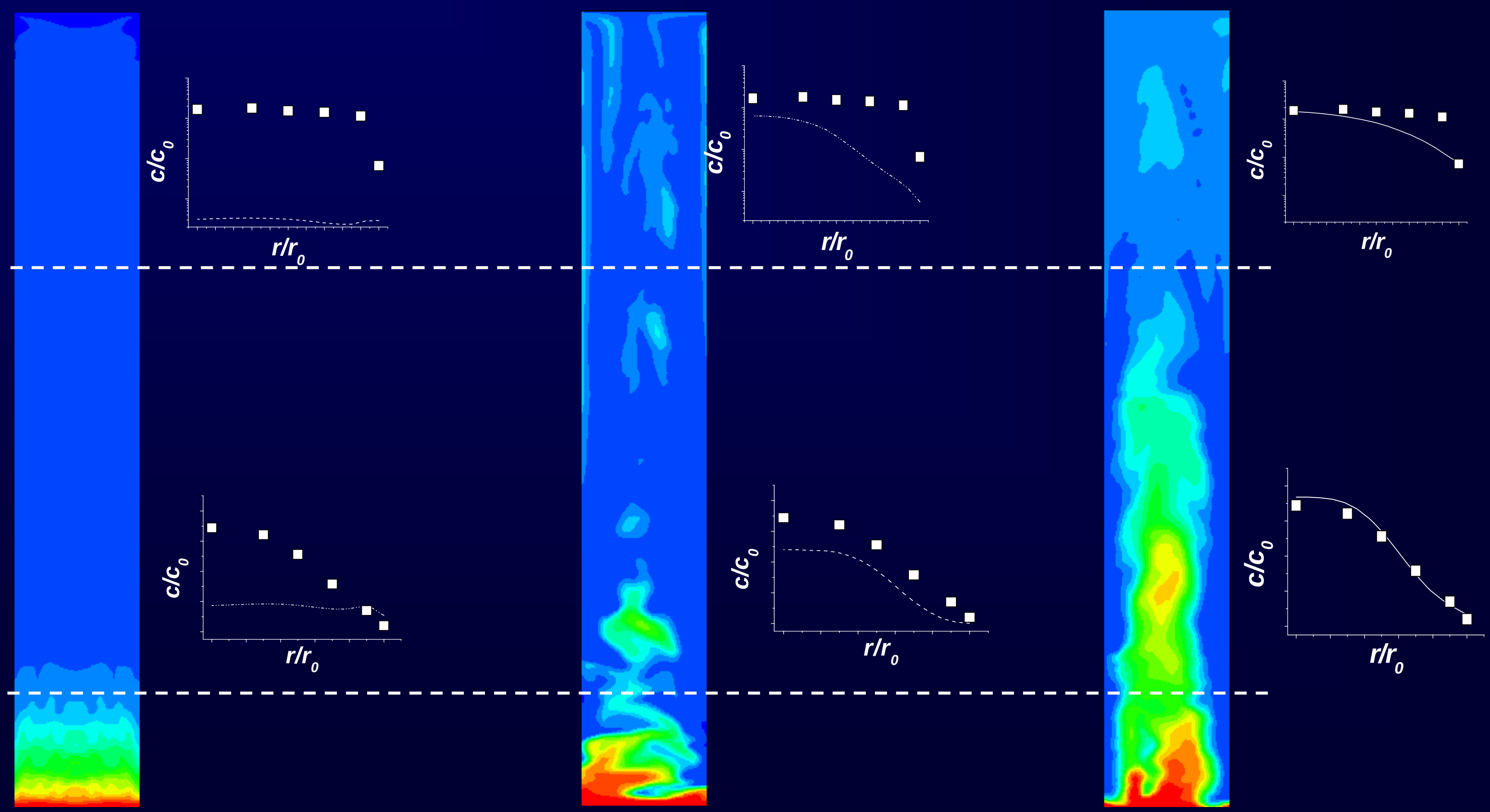
(U_g, G_s) → **Structure-dependent C_D** → **Structure-dependent *Sh***

Comparison between CFD computation and experiments

Averaged flow & averaged mass transfer

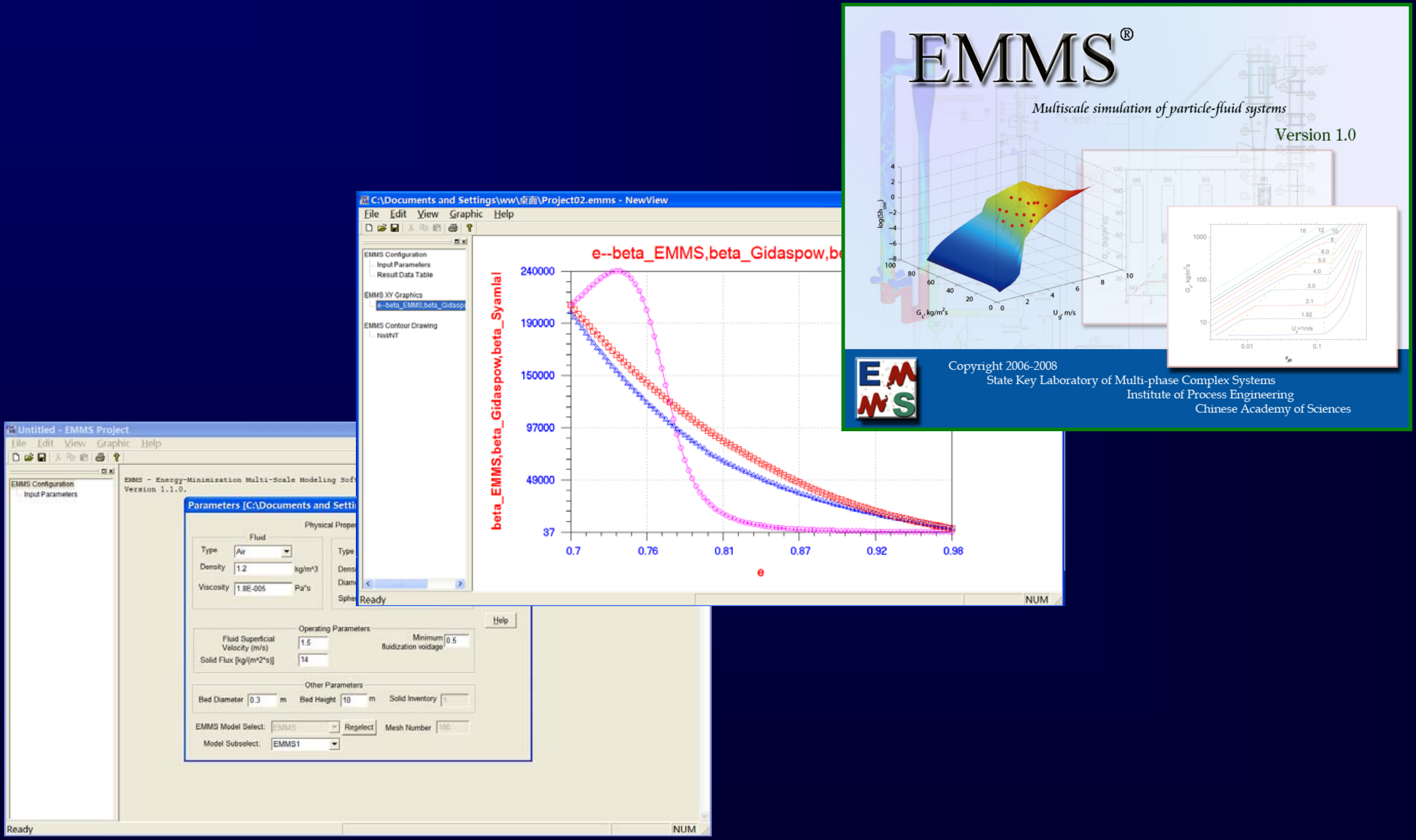
Multi-scale flow & averaged mass transfer

Multi-scale flow multi-scale mass transfer



Dong et al, Chem. Eng. Sci., 63,2008,2798-2823

Commercial codes of EMMS



Applications to industries

SINOPEC Stage 1 :

MIP (max. iso-paraffins) process

Novel FCC Riser

Height: 40 m

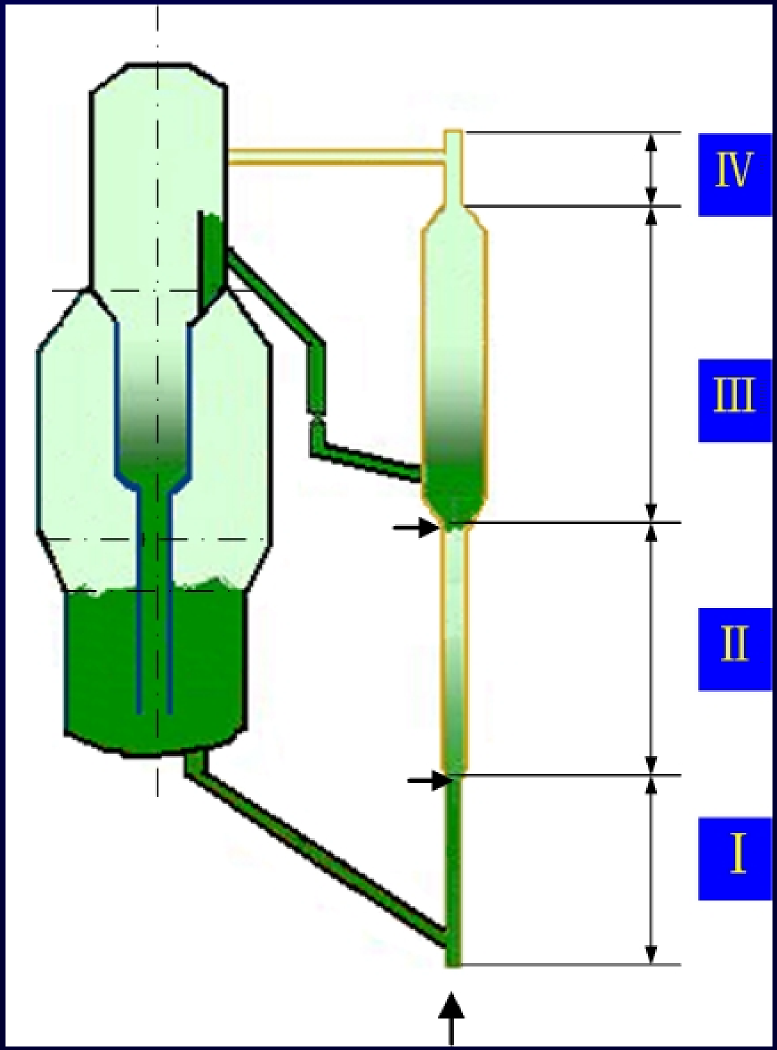
Diameter: 1~3.5 m

Determine design parameter

Diameter

velocity

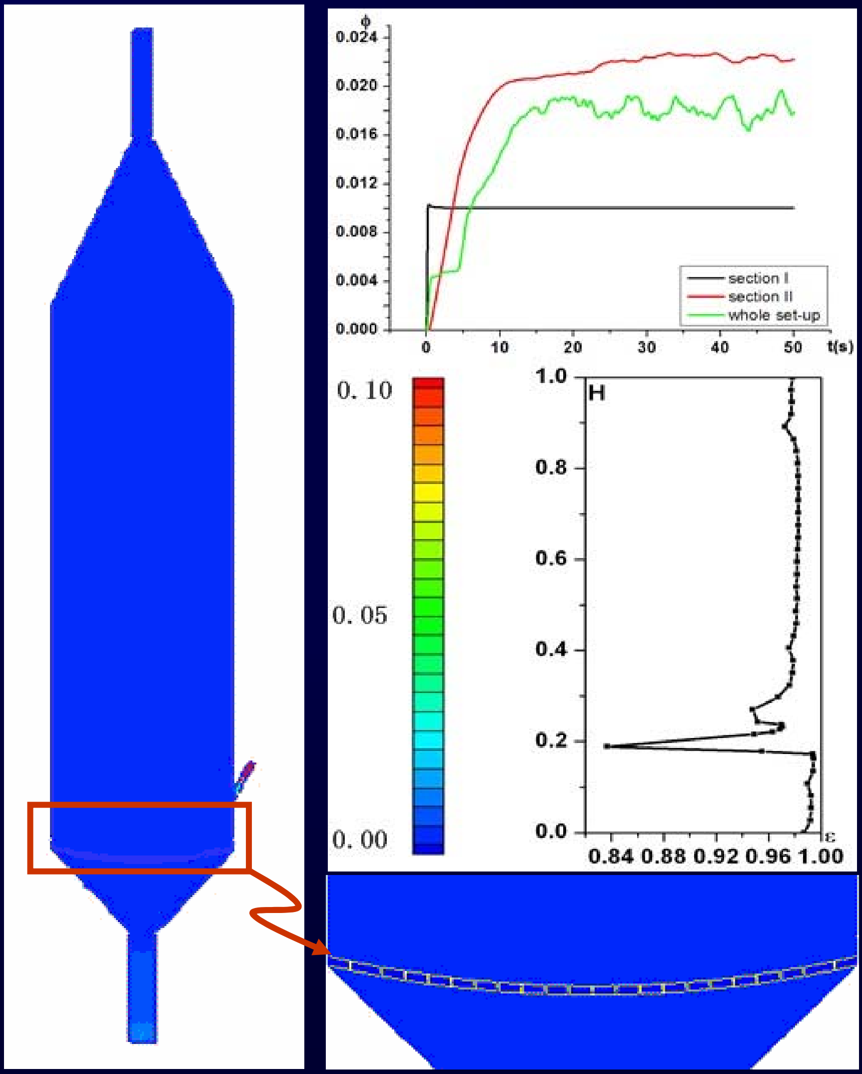
Inventory



Shade of color: concentration

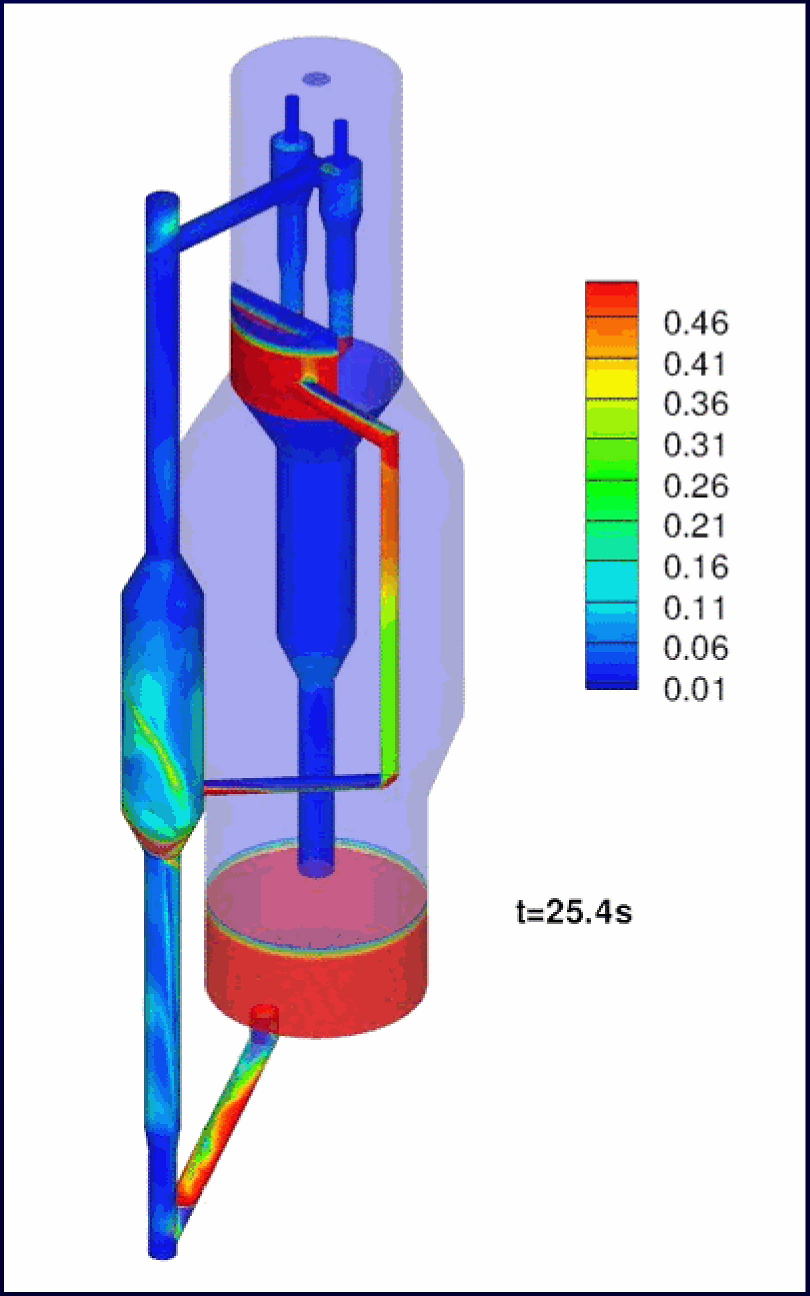
SINOPEC Stage 2 :

Further optimization of MIP process



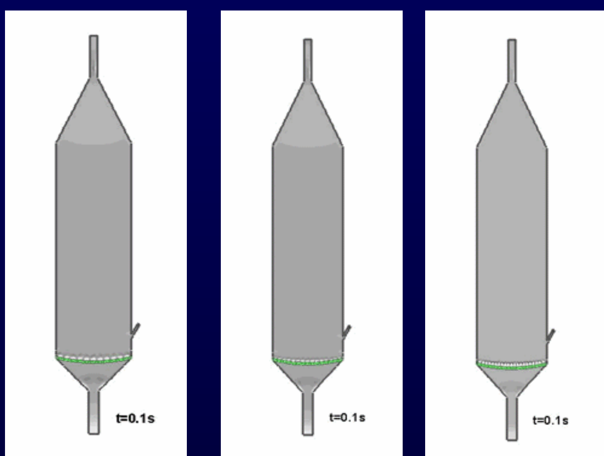
SINOPEC Gaoqiao

MIP process, 1.4 M tons/a



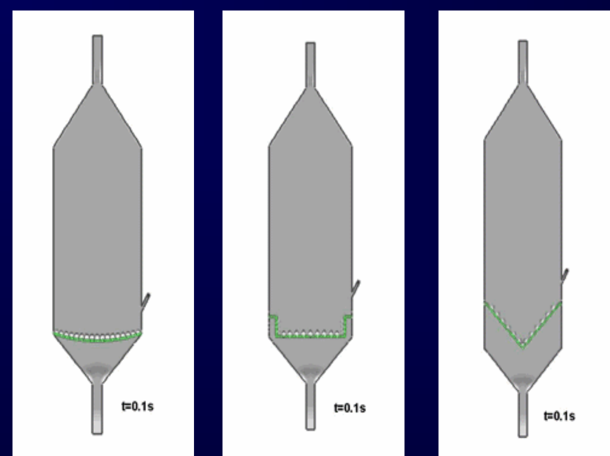
SINOPEC: the influence of

- Orifice number
- Distributor shape
- Outlets



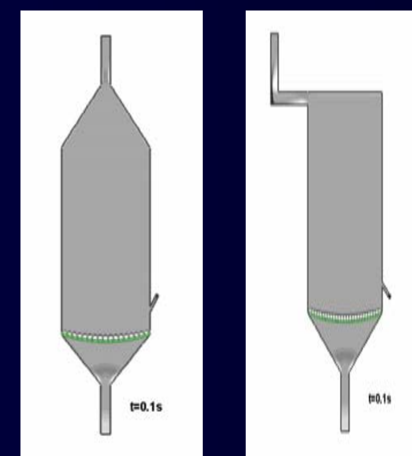
98 169 390

Orifice number



Arc Basin Cone

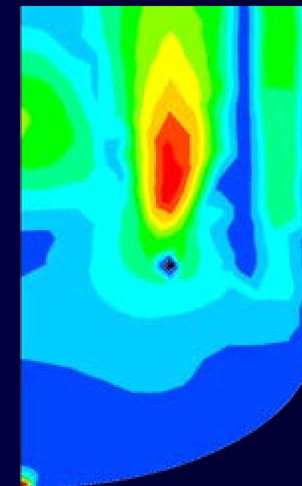
Distributor shape



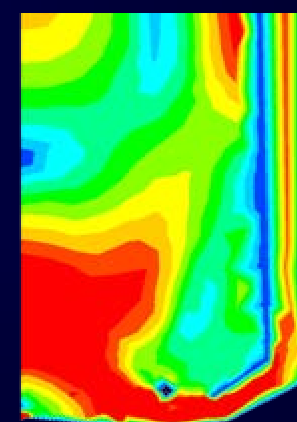
Upright Sideward

Outlet

PetroChina: slurry bed loop reactor



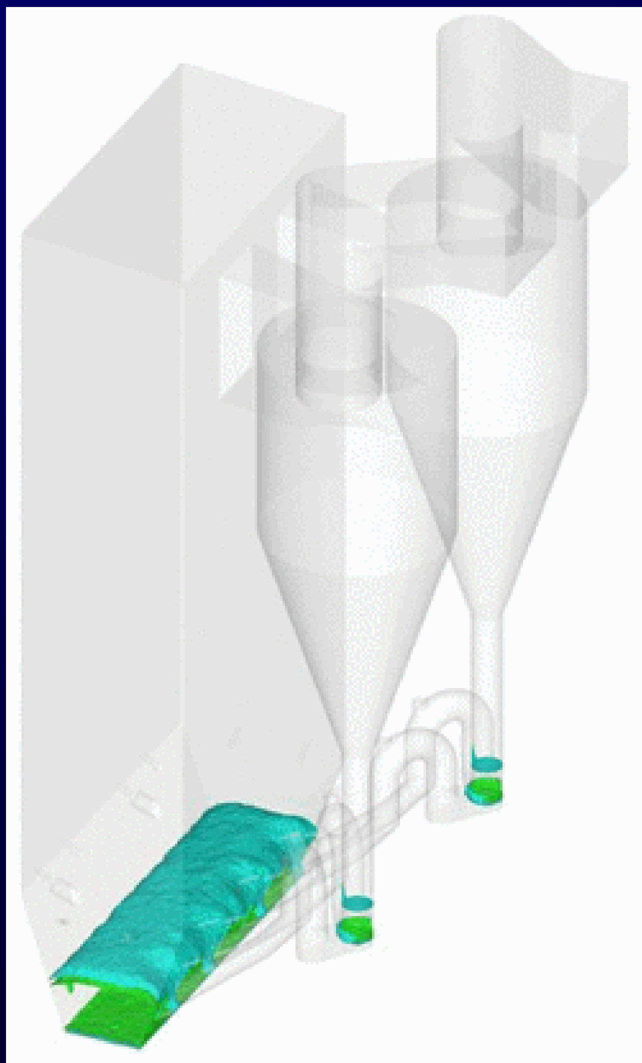
Before optimization



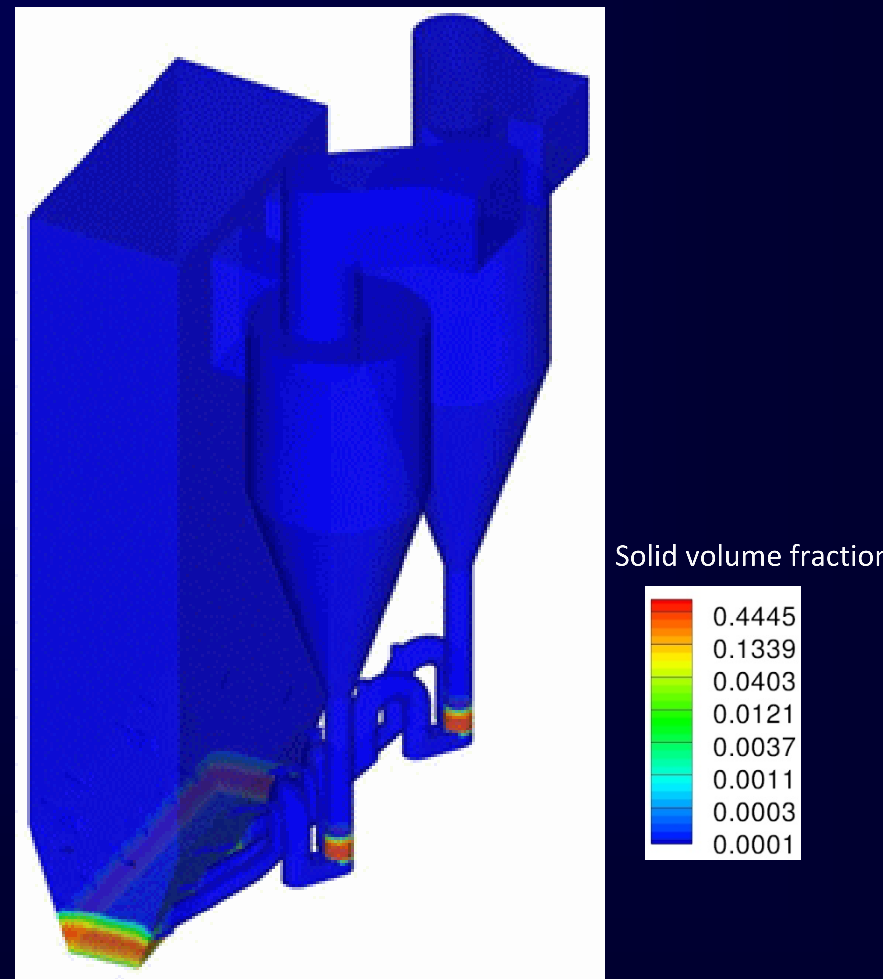
After optimization

Xinhui Power plant

480t/h (150MW)CFB boiler

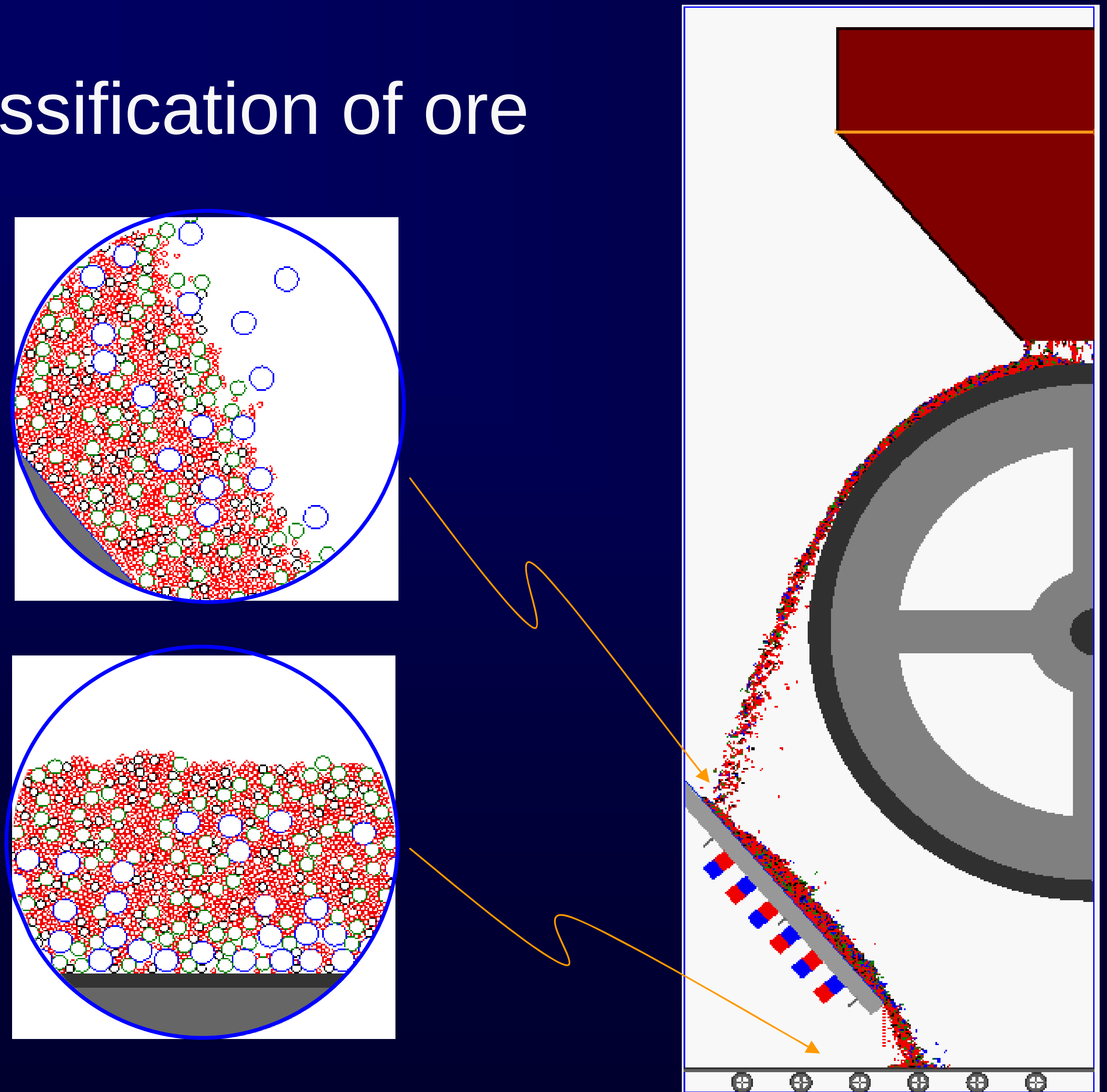


Height:36.5 m
Width:15.3 m
Depth:7.22 m



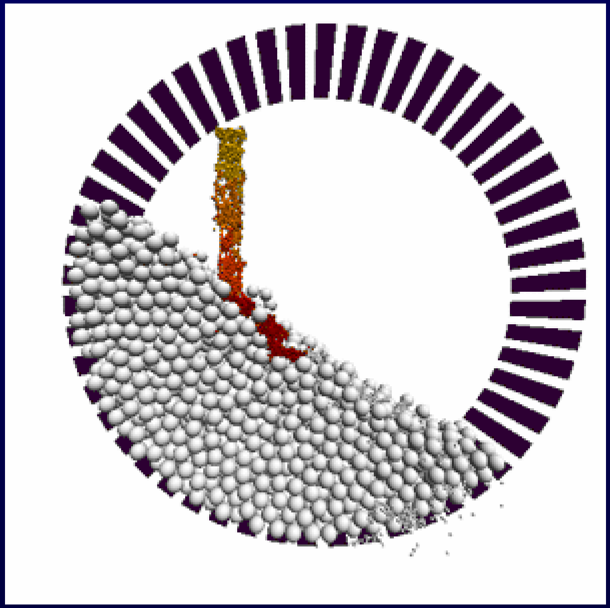
Dispersive particle

Classification of ore

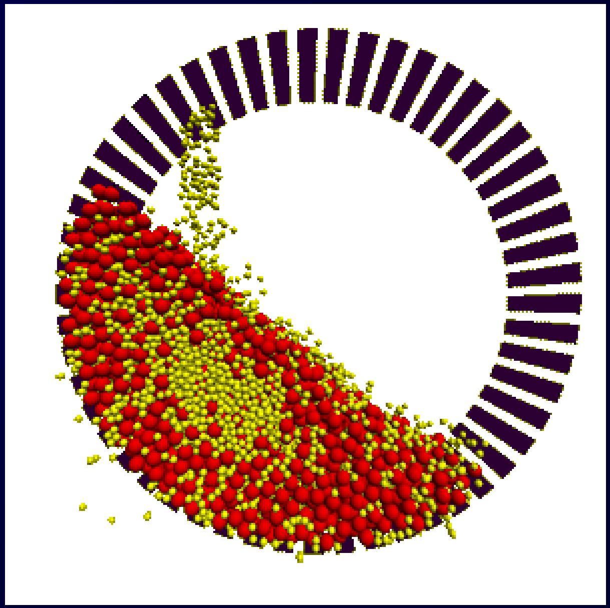


Slag processing in metallugry

Coarse particle → Fine particle/multi particle
1 billion particles

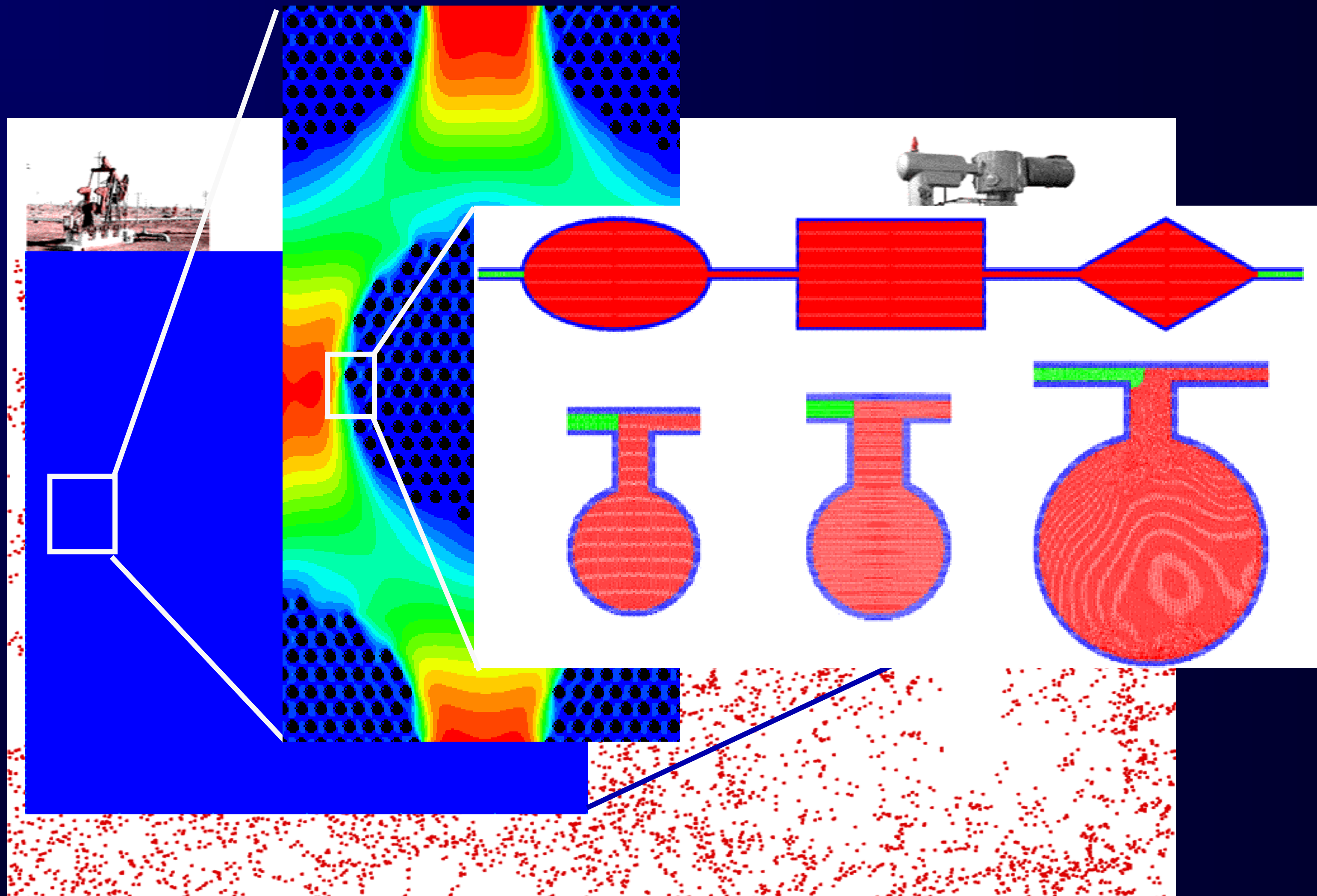


Cool model



Hot model with phase transition

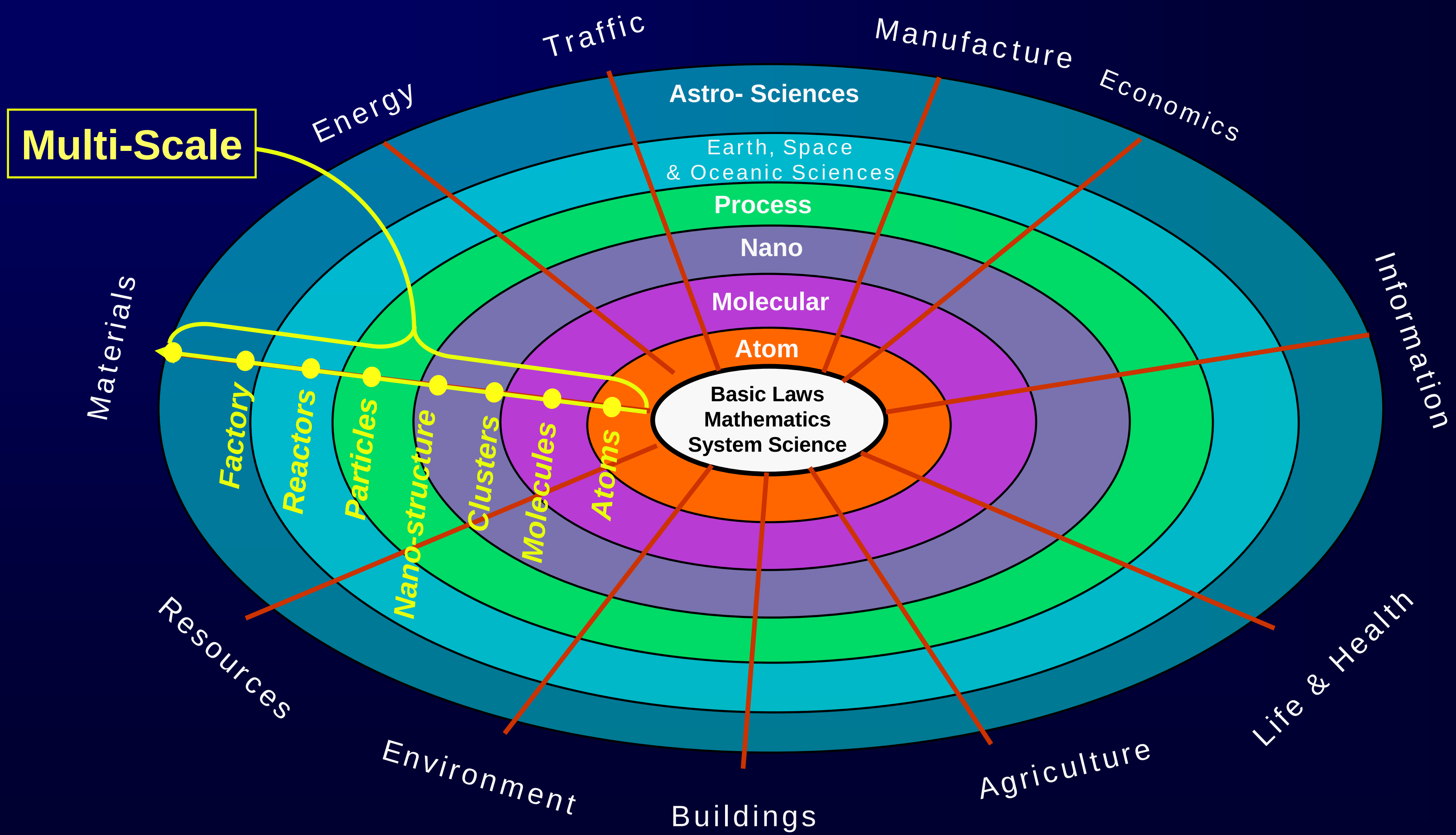
Secondary oil recovery from fractures to oil fields



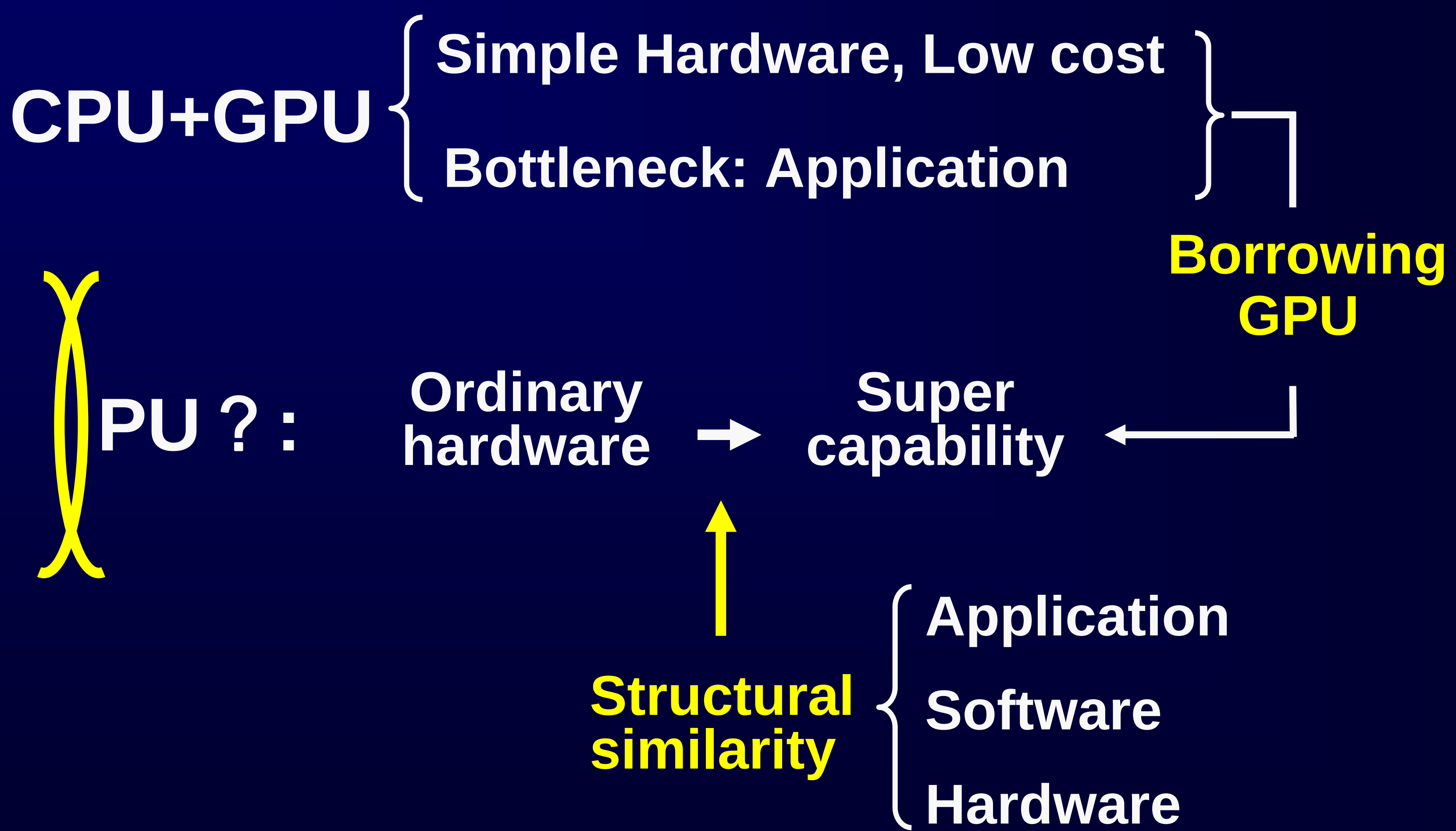
Perspectives

Multi-scale Structure

—— A common challenge for different areas

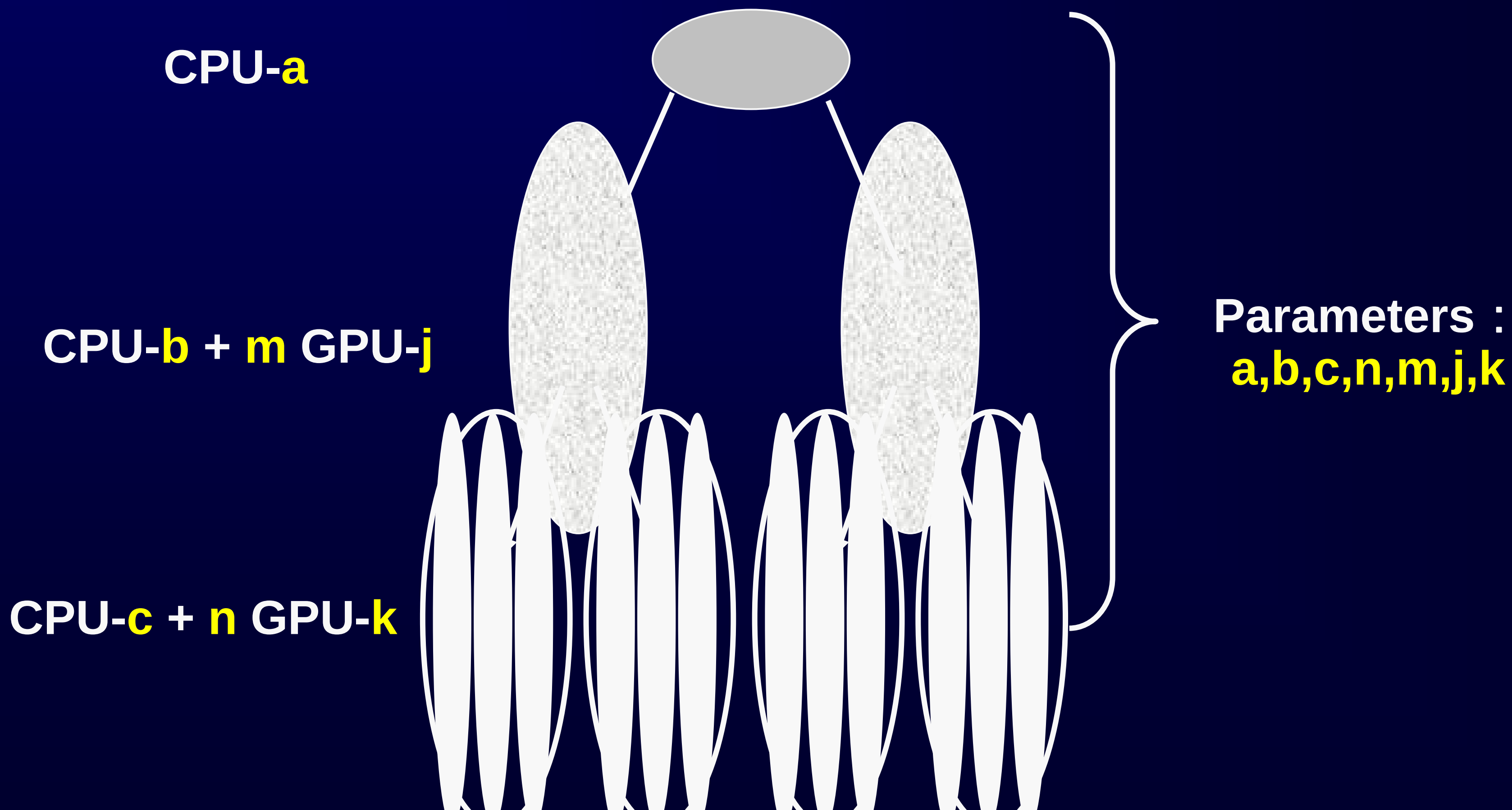


- **Breakthrough of computation capability is expected in near future**



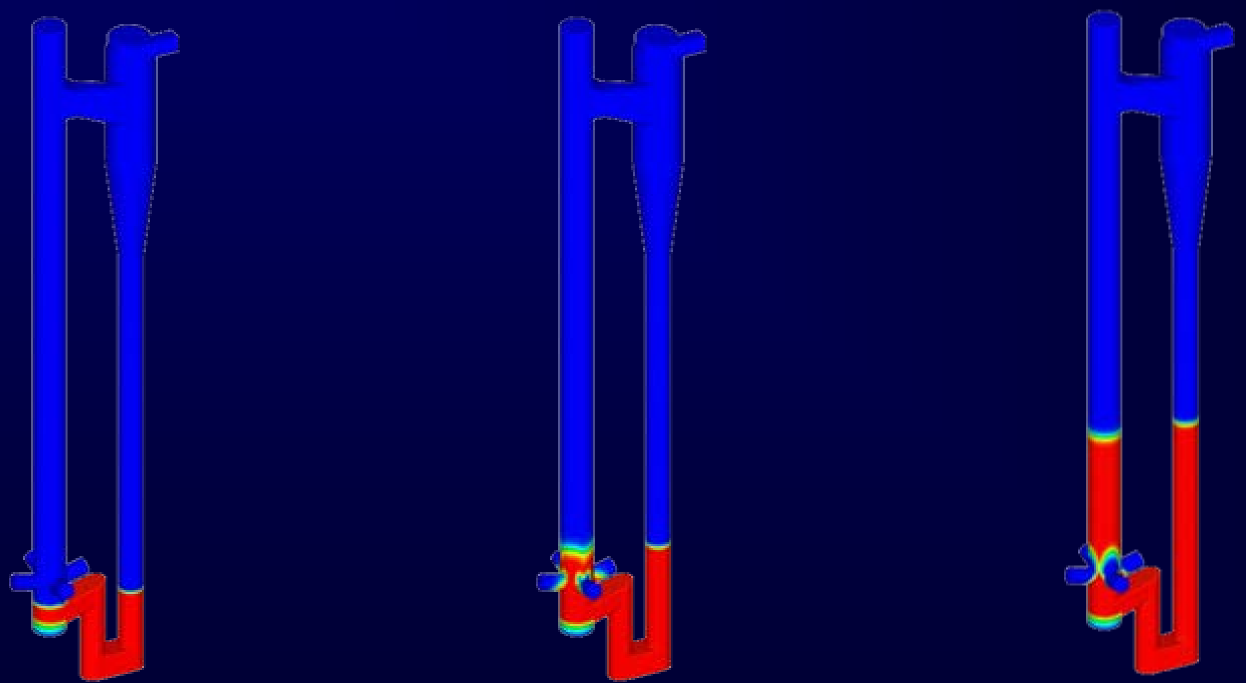
- **Application-oriented**
  - **Hardware→ Software→ Application**
    - Universal
    - Easy to use
  - **Software → Hardware** (Diversity)
    - **High efficiency**
    - **Special purpose**
    - **High cost**
  - **Application**
    - Generality
      - **Common nature → Software→ Hardware**
        - **Conditionally universal**
        - **High efficiency**
          - **Classified design**
          - **Flexible design**
      - **Particularity**

- **Principles for designing variational multi-scale computer systems**



- **Breakthrough in understanding meso-scale structures:**

Virtual Process Engineering: Dream ➡ reality



Ug=3.5m/s → Ug=2.5m/s Ug=2.5m/s

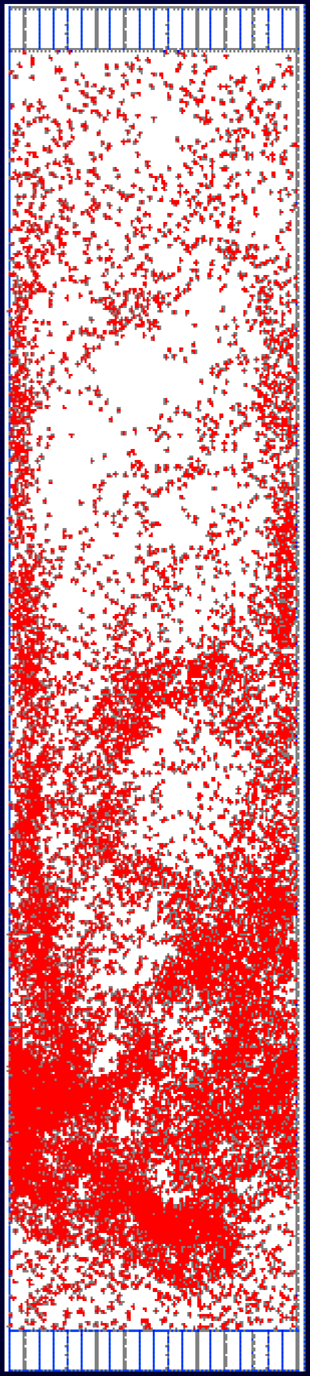
Gs=40 Kg/m^2s Gs=40 Kg/m^2s → Gs=60 Kg/m^2s

Acknowledgement

Supports from: NSFC (Natural Science Foundation of China)
MOST (Ministry of Science and Technology)
CAS (Chinese Academy of Sciences)

Coworkers:

Thanks for
your attention !



Retrospect and prospect: