Last update: May 17, 2010

Multi-Scale Discrete Simulation on Multi-Scale HPC System

Group of Complex System and Multi-scale Simulation
Institute of Process Engineering, Chinese Academy of Sciences
Presented by *Wei Ge*

Outline

Challenges and approaches

Software and hardware development

Applications in different areas

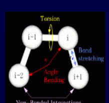
Summary and prospects

Multi-scale simulation in process engineering

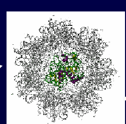
Can we find an accurate, efficiency and general way ?

Toooo… costly!

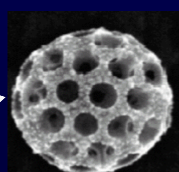
MD



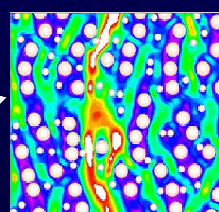
MC / DPD



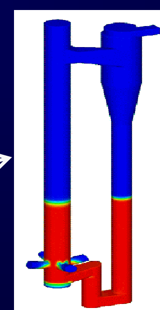
DEM



PBM



TFM



Flow sheet

Agent

Angstrom	nm	µm	mm	m	km	Mm
fs	ps	µs	ms	s	hour	year

molecule

molecular cluster

particle

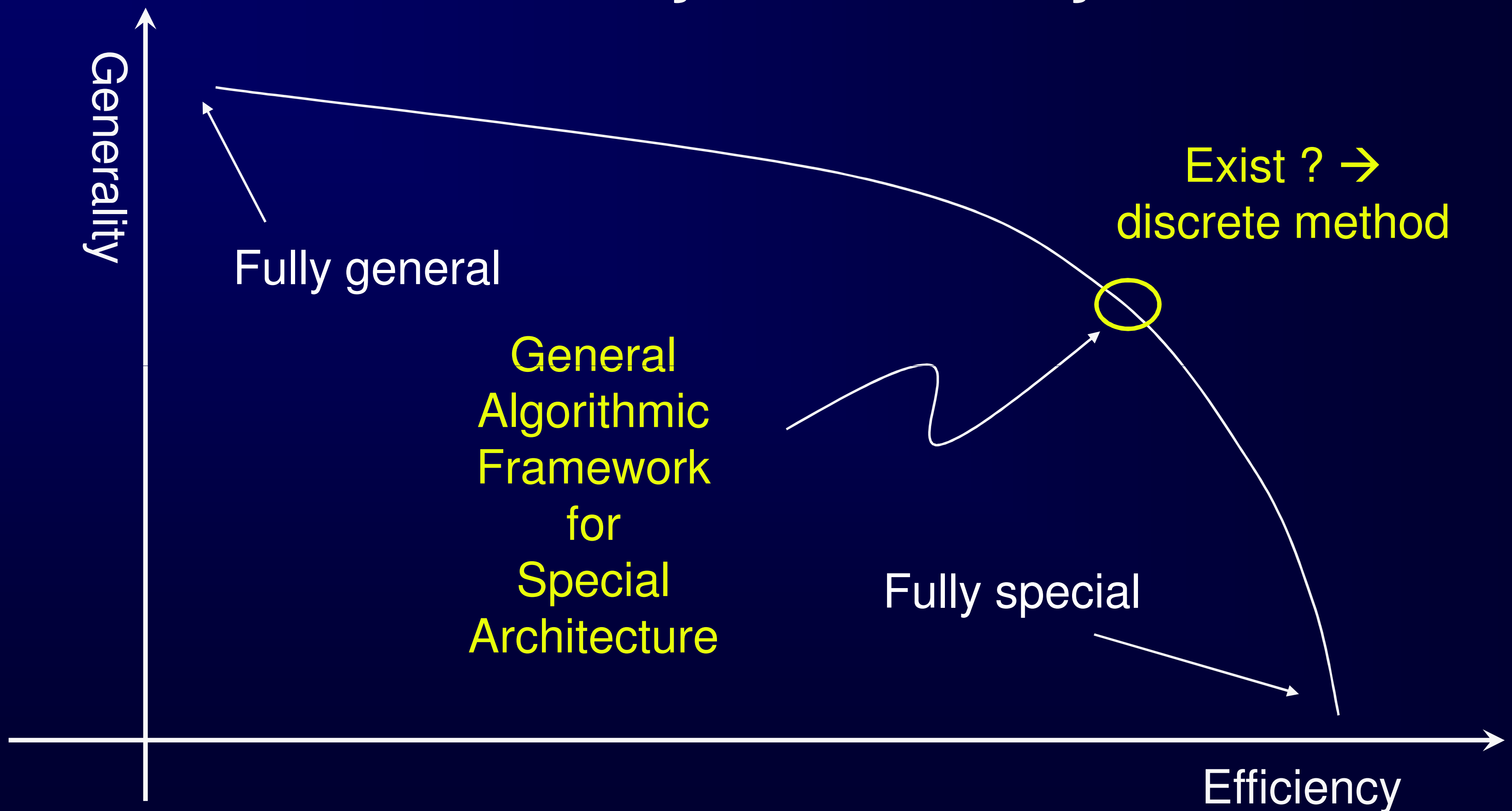
particle cluster

reactor

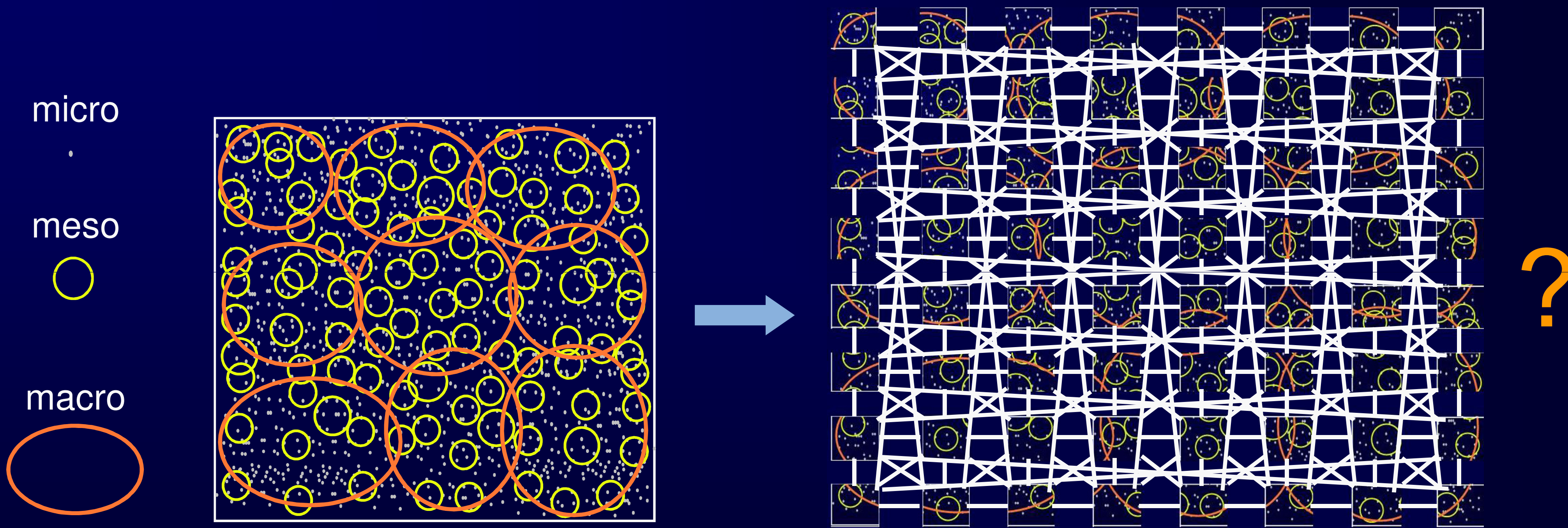
process

environment

Generality vs Efficiency



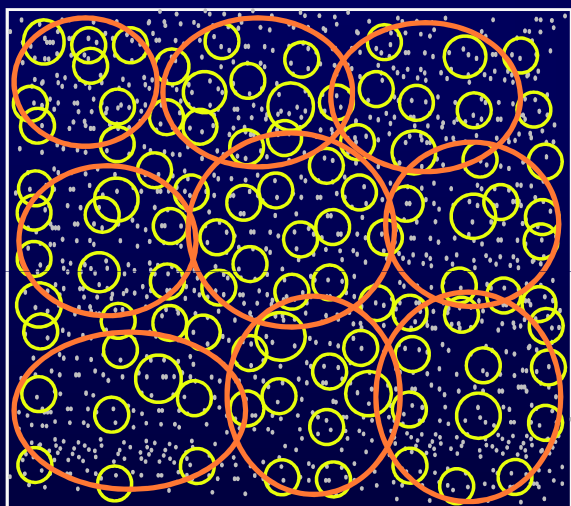
Traditional parallelization



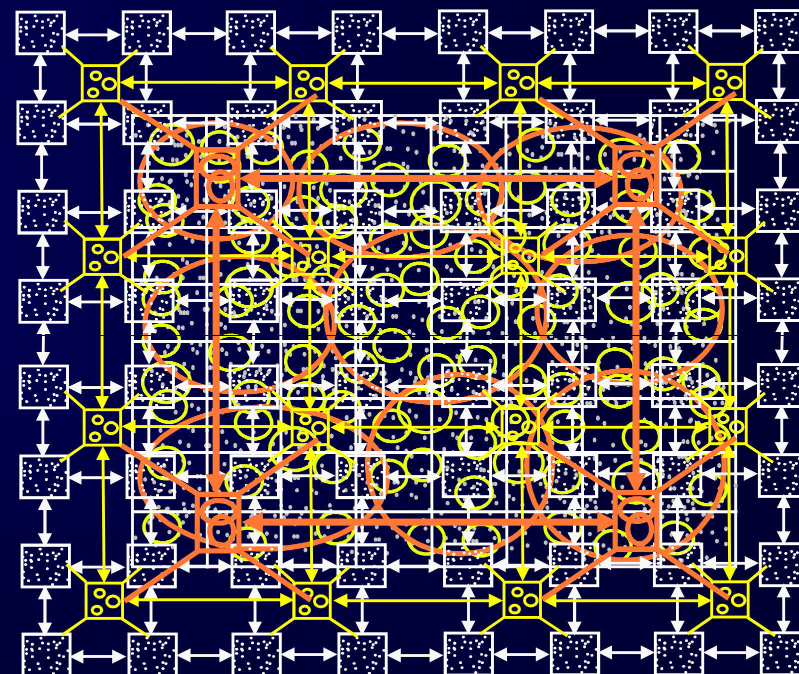
Multi-scale world

Global communication,
Mono-scale parallelization

Multi-scale parallelization



Multi-scale world



Local communication,
Multi-scale parallelization

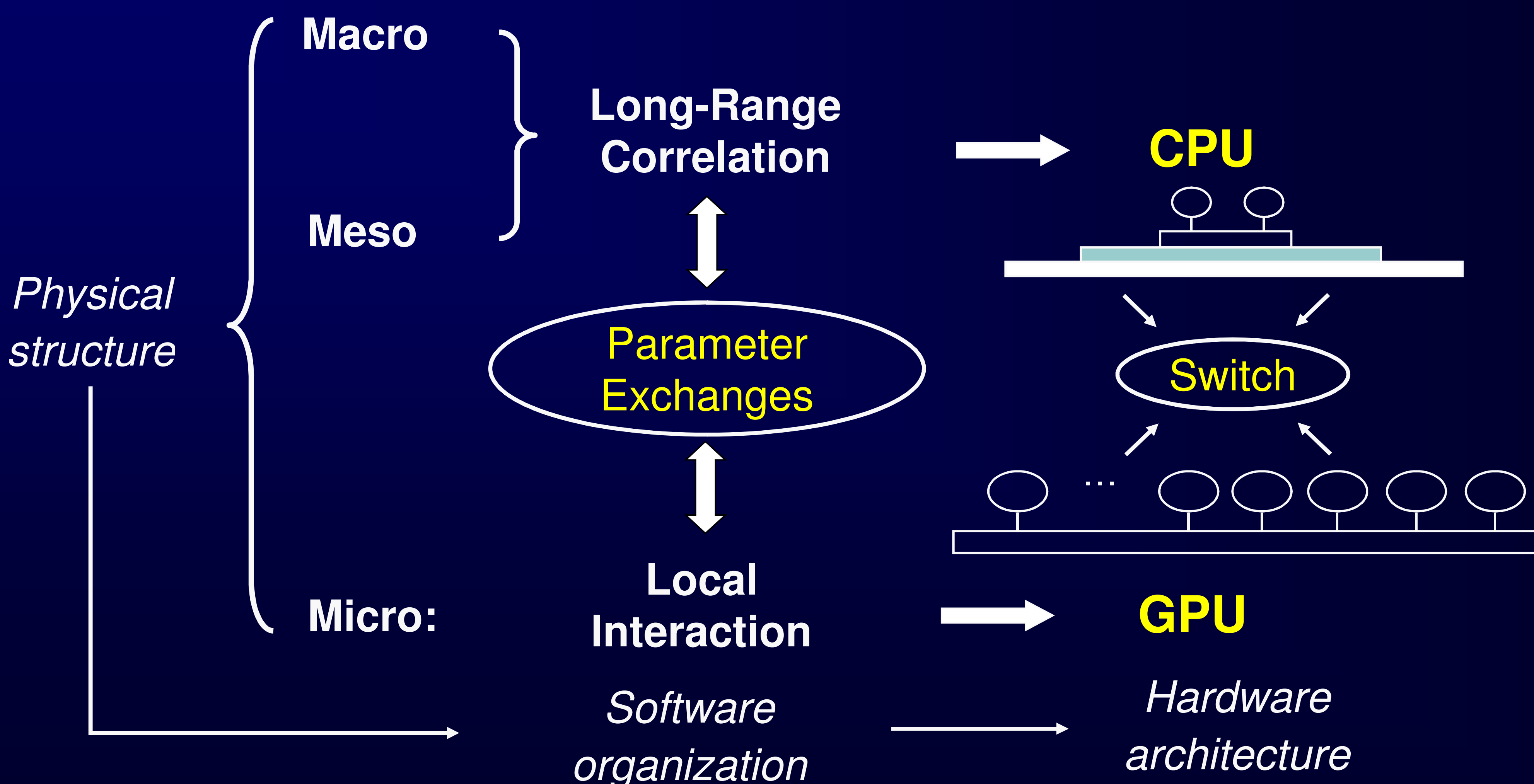
Hierarchy of discrete approaches for complex flows

Micro-scale: fluctuating, conservative
MD, DSMC, LGA, PPM, …

Meso-scale: fluctuating, dissipative
DPD, FPM, DSPH, LBM, …

Macro-scale: smooth, dissipative
SPH, MPS, DEM, MaPPM, …

Consistency: Physics, Algorithm, Architecture



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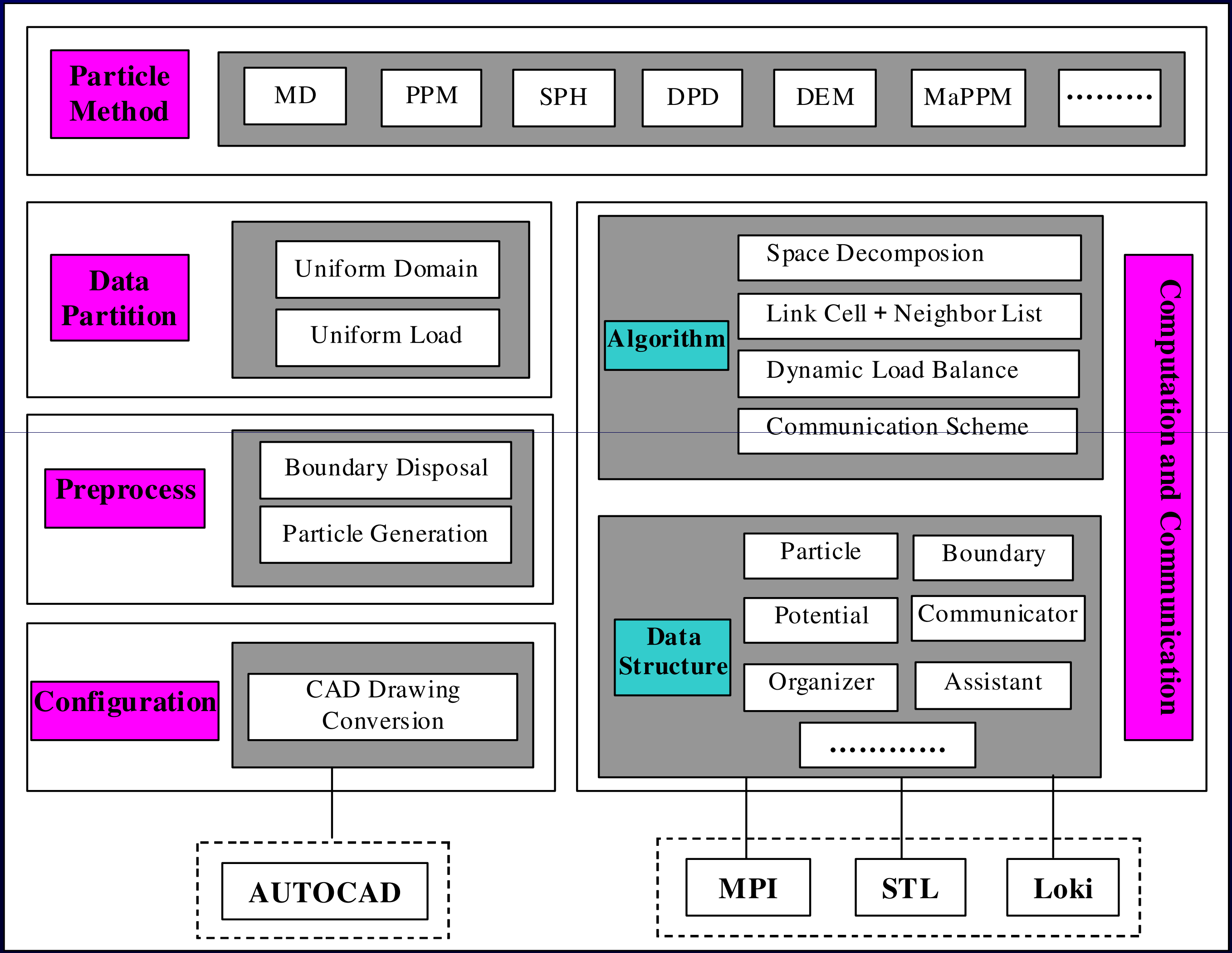
General Platform for Discrete Simulation

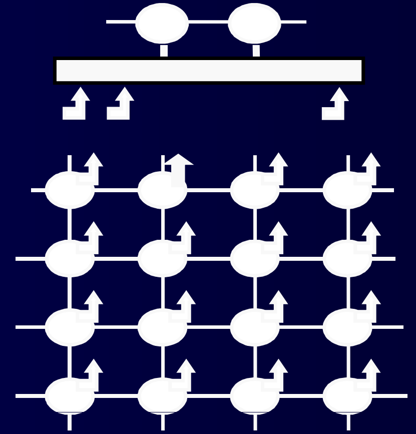


C&CE, 2005, 29:1543-1553;

Ge et al., Sci. in China, 2005

100Tflops GPU system (2008.2.18)

R_peak :	127Teraflops SP
Nodes :	126×HP8600
CPU :	252×Intel 2.66GHz
GPU cards :	200×NV Tesla C870 +20×NV GeForce 9800×2
Network :	Gigabit Ethernet (mesh+tree)
Switch :	H3C 7506R
OS :	RedHat Linux 5.2
R_real :	20 ~ 40Tflops

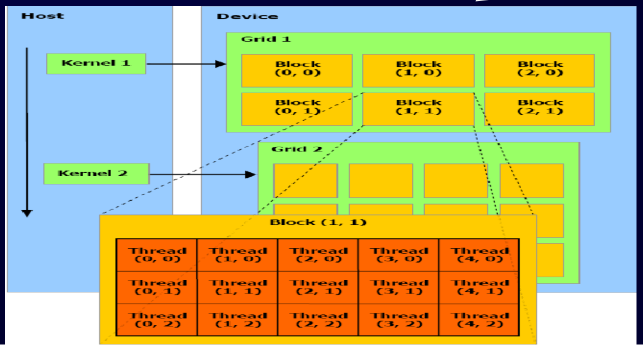


2×3

10×12

6.023e(23-9.7)
flops

Mole-9.7
(<70kW)



China's first HPC system with 1.0 Petaflops peak performance in single precision (2009.3.19)

2x48x GE SW — 4x — 288x GE SW

84x	32x	52x	32x	128x
Top + Middle 2x4C+HD4870x2 201.6T	Middle 4C+2xC1060 64T	Bottom 4C+3xG280 140.4T	Bottom 4C+2xHD4870x2 153.6T	Top + Bottom 2x4C+2xG295 460.8T
84x	32x	52x	32x	128x

2x48x IB-DDR SW — 4x — 288x IB-DDR SW

200T(IPE/Dawning)

200T(IPE/Lenovo)

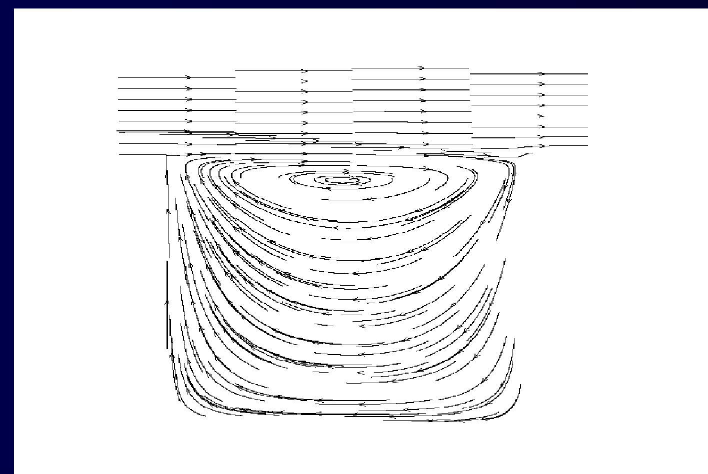
150T(IPE)

450T(IPE)

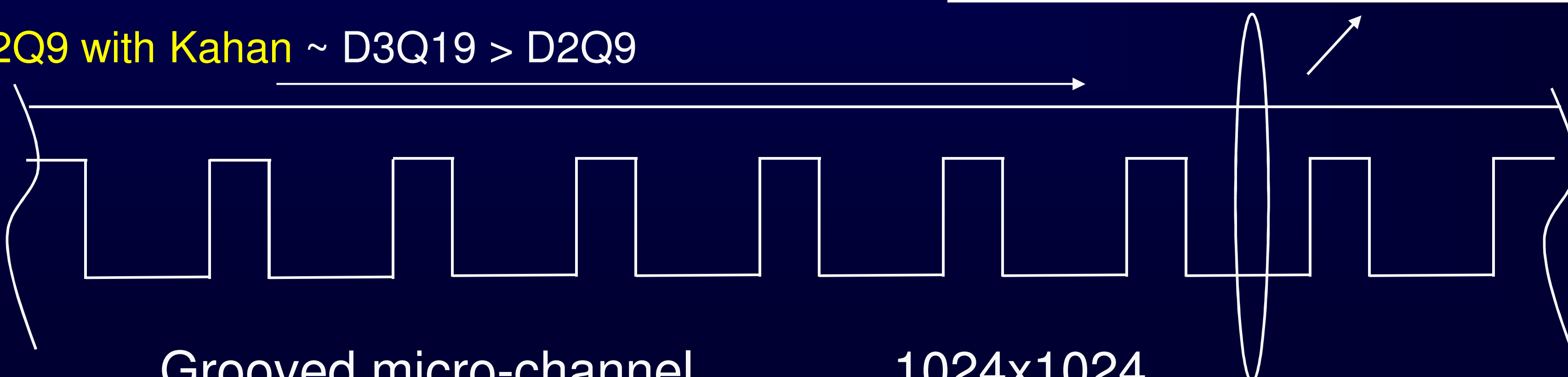
Mole-8.7 (<300kW)

Real performance in Couette-cavity flow

Scale	Tflops(sp)	Efficiency
464GT200	163.3 / 432.9 (288.6)	39.4% (59.1%)
120RV770	24.9 / 144	17.3%
680GT200+ 274RV770	118 / 963 (306)	12.5% (31.7%)



D2Q9 with Kahan ~ D3Q19 > D2Q9



Grooved micro-channel 1024x1024

First Fermi-based GPU supercomputing system

2010.04.24

Rpeak SP :	2Petaflops
Rpeak DP :	1Petaflops
Total RAM :	17.2TB
Total GRAM :	6.6TB
Total HD :	360TB
Data Comm. :	Mellanox QDR InfiniBand
Inst. Comm. :	H3C Gigabit Ethernet
Occupied area :	$150m^2$ (with internal cooling)
Weight :	12.6T (with internal cooling)
Max Power :	600kW(computing)+200kW(cooling)
System :	CentOS 5.4, PBS
Monitor :	Ganglia， GPU monitor
Languages :	C，C++，Fortran，CUDA ，OpenCL

Distributed GPU-Supercomputing in China

Collective capacity：

4.907Petaflops SP

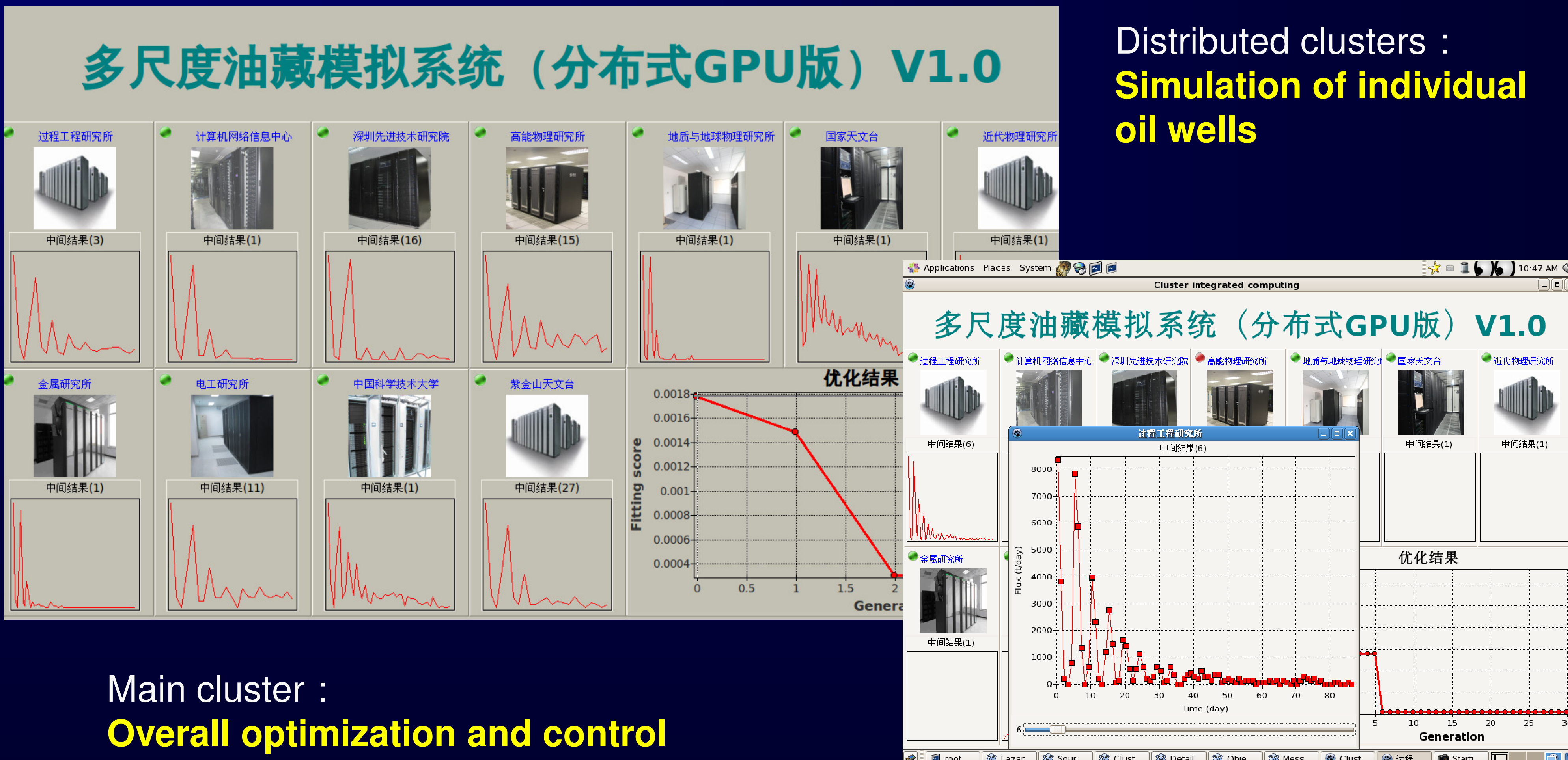
1.300Petaflops DP

IPE Mole-8.5

3Petaflops SP，1Petaflops DP

过程所	高能所	金属所	深圳先进院	国家天文台	地质地球所	网络中心	近代物理所	紫金山台	电工所	中科大
NV+AMD	AMD	NV	NV	NV	NV+AMD	NV+AMD	NV	NV	NV	NV
1P SP	200T SP	183T SP	173T SP	160T SP	200T SP	300T SP	202T SP	183T SP	101T SP	205T SP
100T DP	40T DP	15T DP	14T DP	13T DP	17T DP	39T DP	17T DP	15T DP	8T DP	17T DP

Distributed GPU computing for oil recovery



Distributed clusters：
Simulation of individual oil wells

Main cluster：
Overall optimization and control

Outline

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Multi-scale: from method to hardware
Applications in different systems
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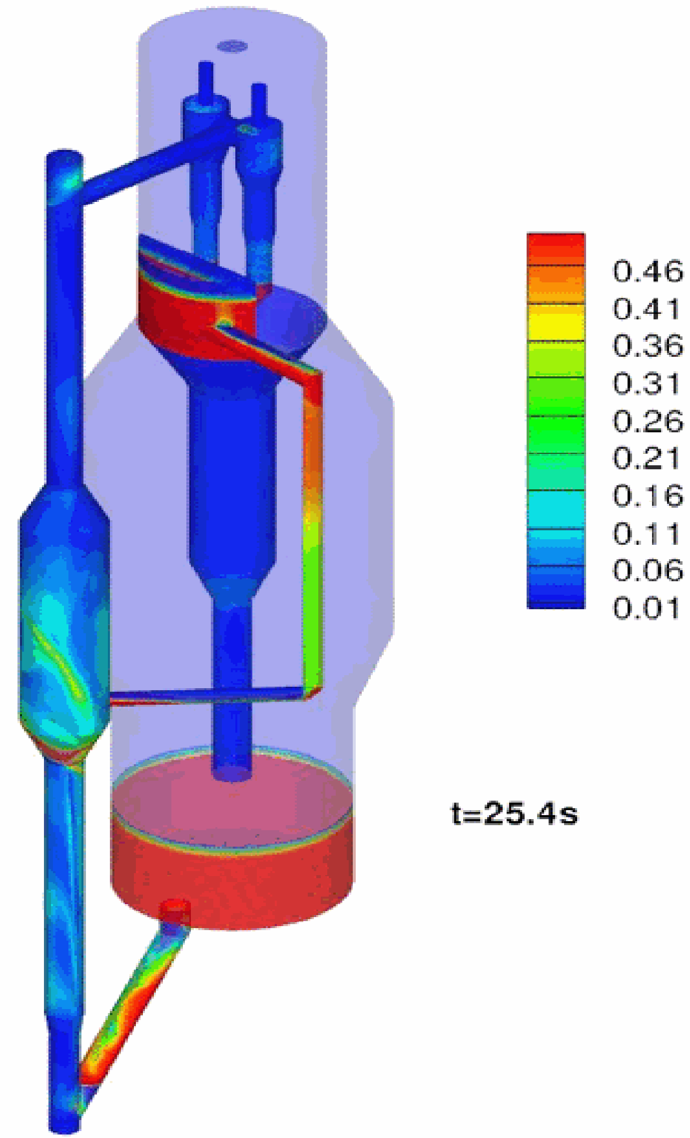
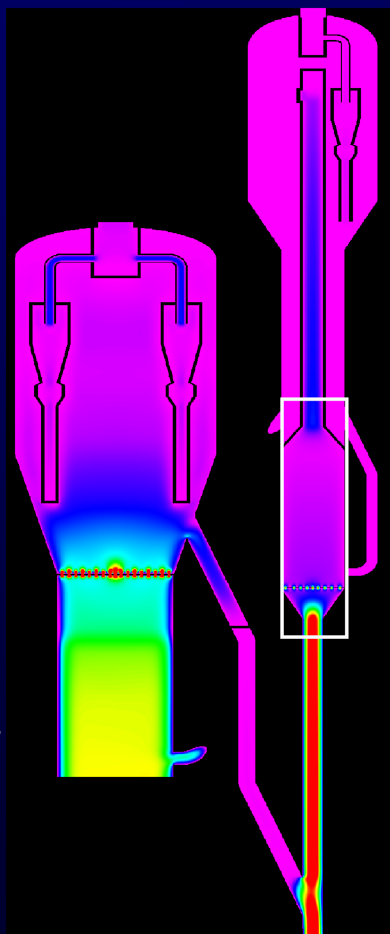
Case study: Oil refining

1.4Mt/a MIP FCC process producing 1/3 gasoline in China



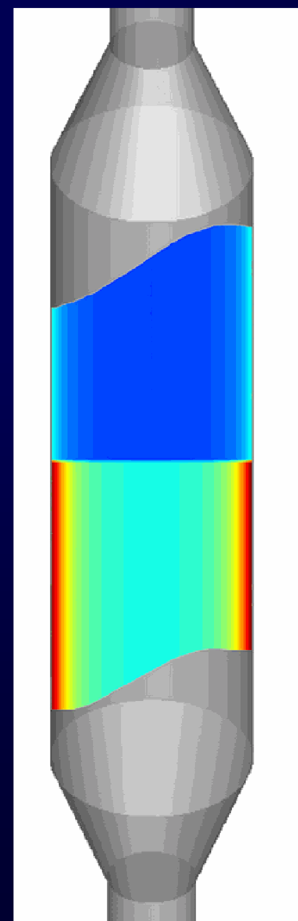
Simulation of gas solid flow on multi-scales

Reactor:
9*40m
3D
EMMS



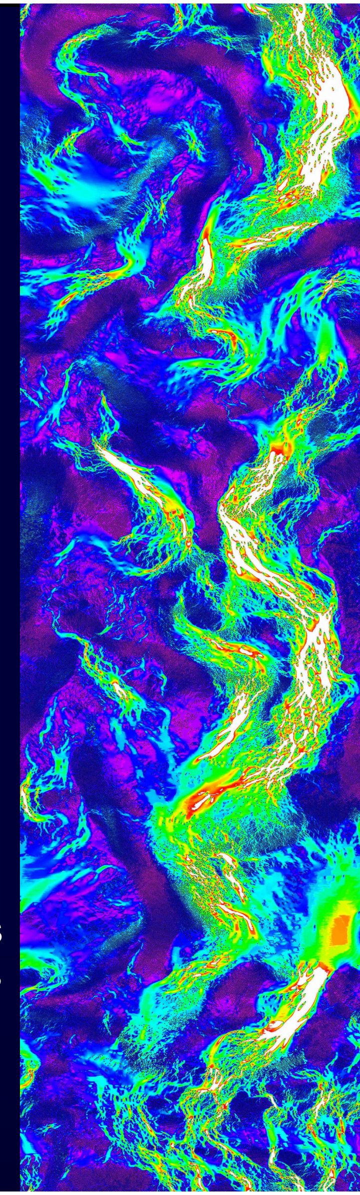
100M grids
432 GPUs
~3s
~100x
speedup

Section:
3*10m
2D
CFD+
EMMS



1.2M cells
96 GPUs
Realtime
~50x
speedup

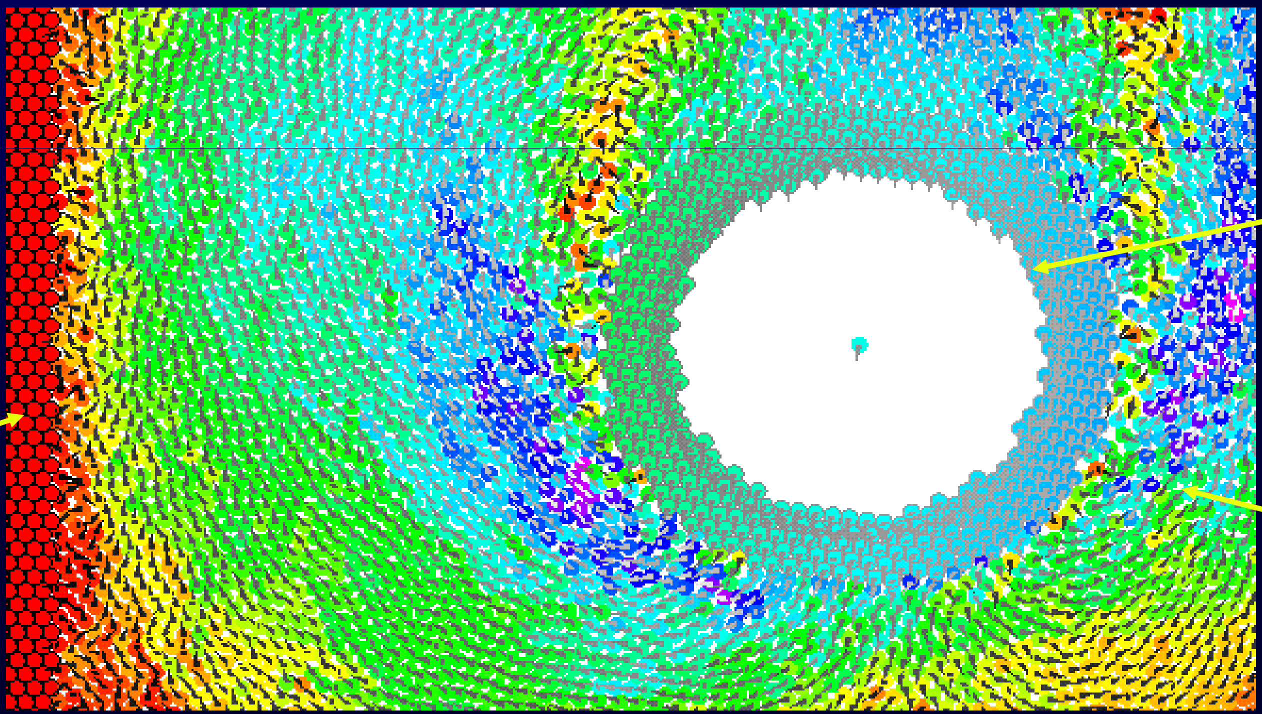
Cell:
2*10cm
2D
DNS in
MaPPM



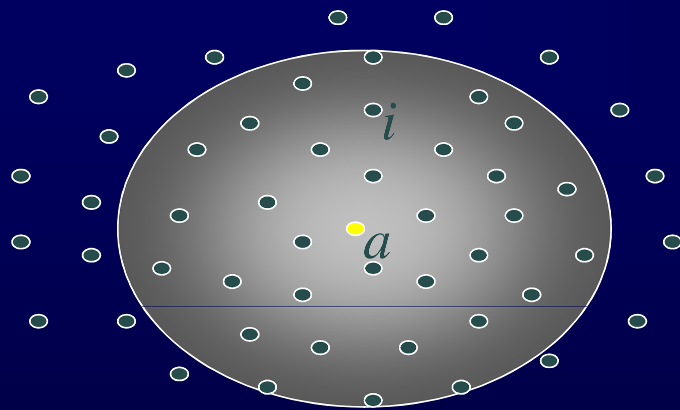
120k solids
~ 1G fluids
144 GPUs
20~30x
speedup

Approach: Particle-fluid flow → particle-particle flow

	Particle	**Continuum**
Velocity difference →	tangential stress	viscosity
Density difference →	normal stress	pressure



A straightforward formulation



$$\nabla f\,|_a = D\sum_i \frac{f_{ia}}{r_{ai}^{\;2}}\boldsymbol{r}_{ai}\frac{m_i}{\rho_i}W_{ai}$$

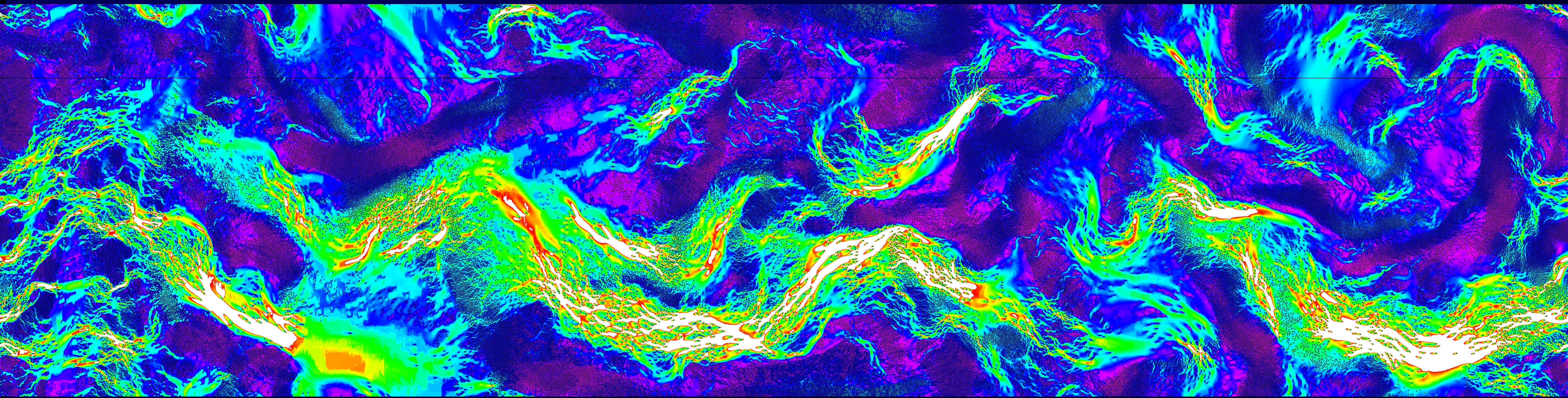
$$\Delta \boldsymbol{f}\,|_a = 2D\sum_i \frac{\boldsymbol{f}_{ia}}{r_{ai}^{\;2}}\frac{m_i}{\rho_i}W_{ai}$$

Ge & Li, 2003, Powder Tech. 137:99

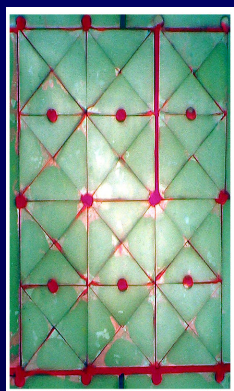
Animation Challenge:

9600x2400 → 1200x300 pixels

1000 → 17 frames

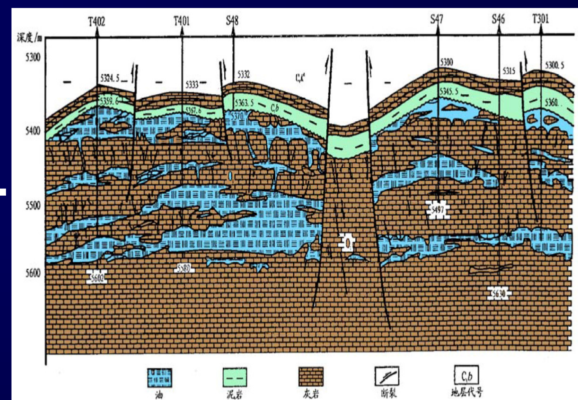


Oil recovery: fracture-cave type oil fields



Physical Experiment

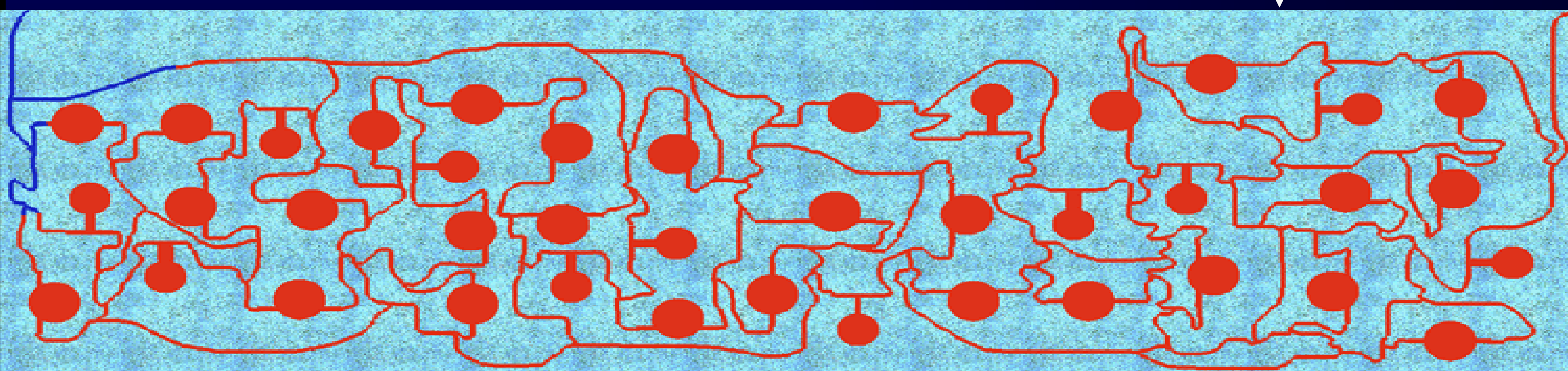
0.5x0.8m
days



Geological Structure

20x20km
years

Simulation
80 GPUs
500x150m
Month
(in hours)



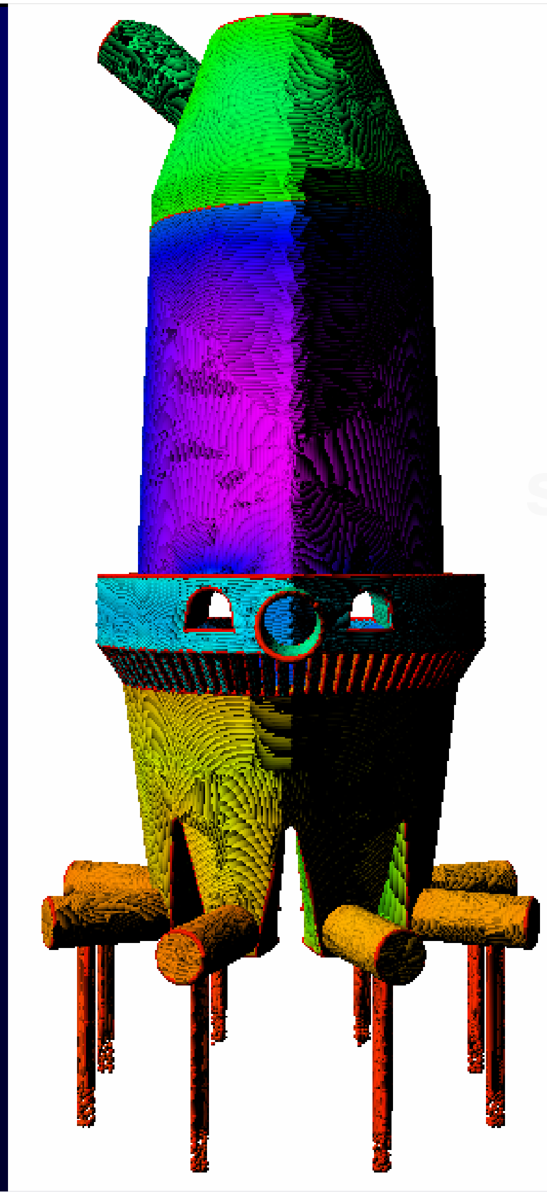
Metallurgy:

new

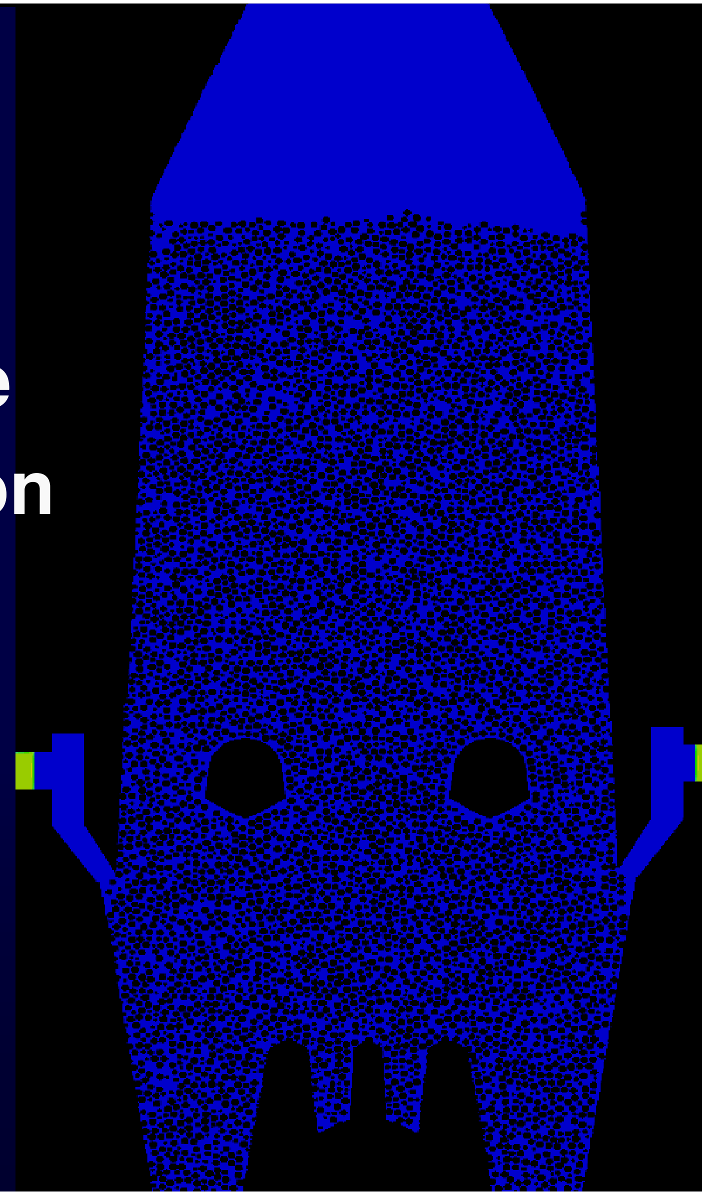
process

“COREX”

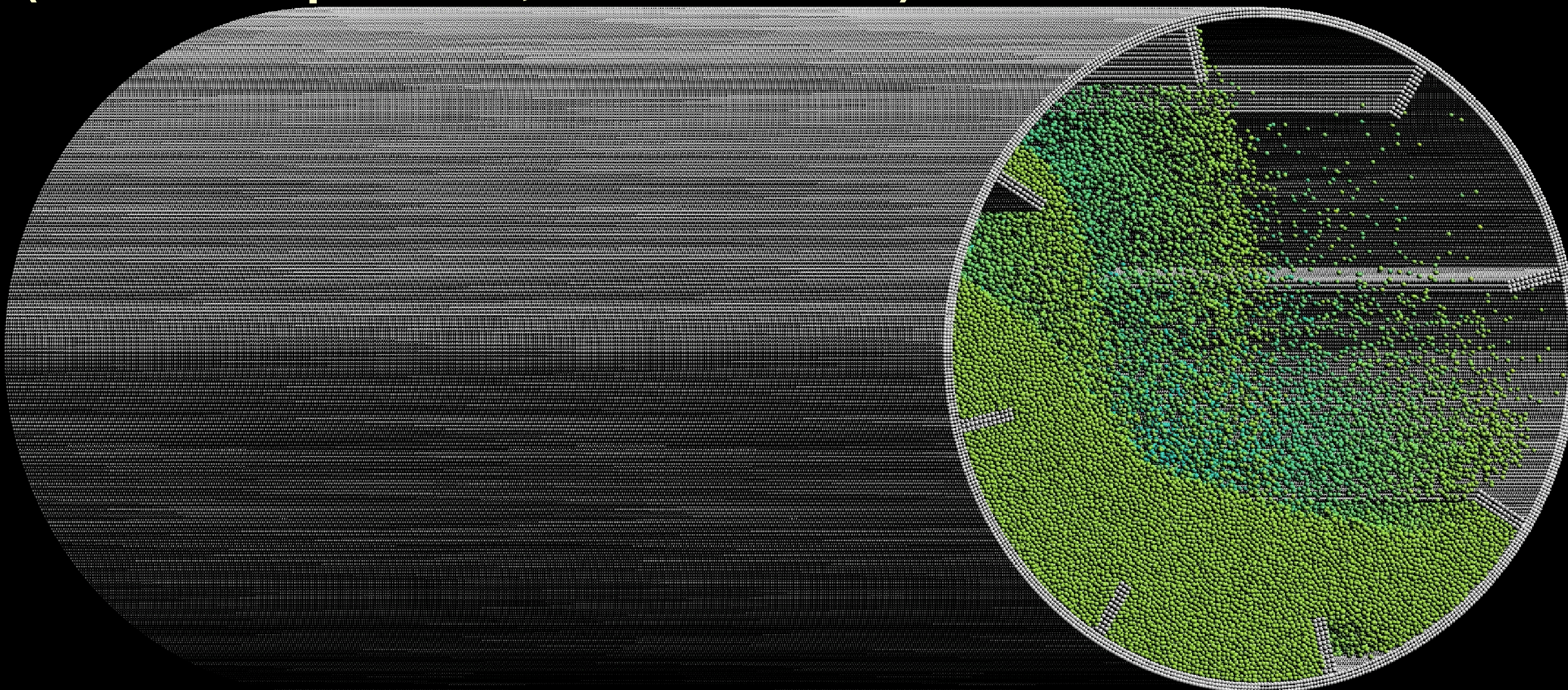
30x9m



Flow in porous media: realtime simulation

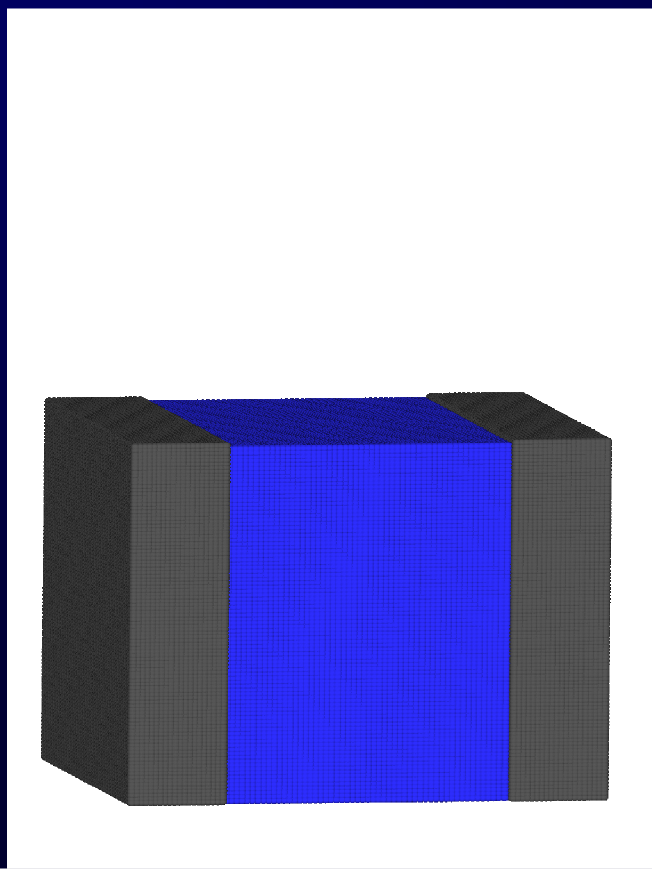


Particle handling: real time simulation of a rotating drum
(9.6 million particles, 13.5*1.5 meter)

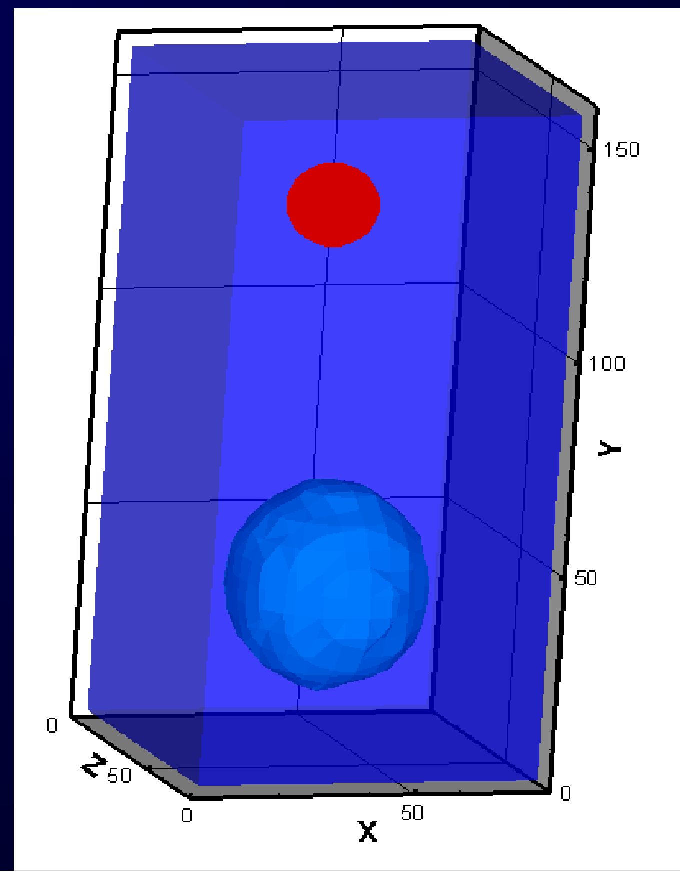


Micro-/Nano-fluidics:

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
15~50x speedup

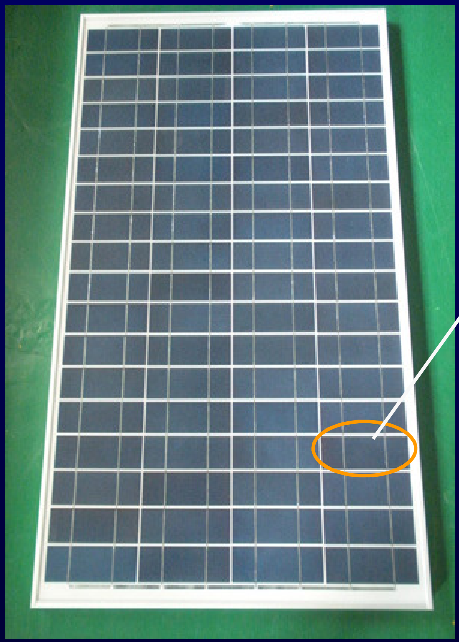


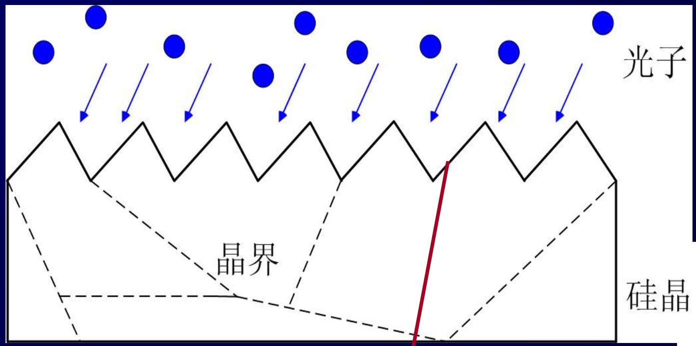
3D simulation: gas-liquid phase transition
0.1*0.05*0.1µm,
LJ/PP fluid at 60K, NVT ensemble
1M particles, 2GPU

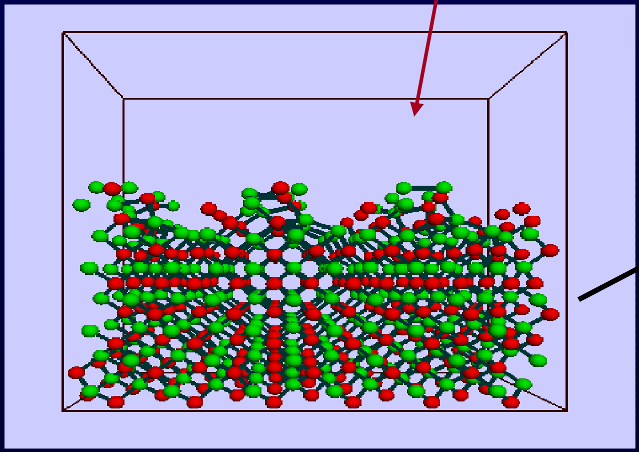


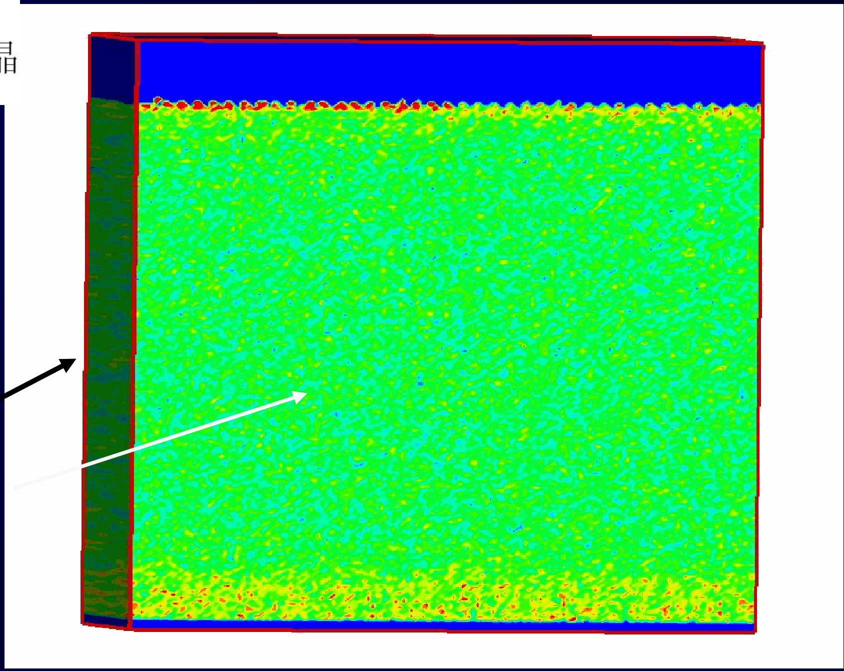
Material : multi-scale structure in solar cells

43.2nm x 48.7nm x 5.4nm
572,800 atoms
1GPU, 50x speedup, for force

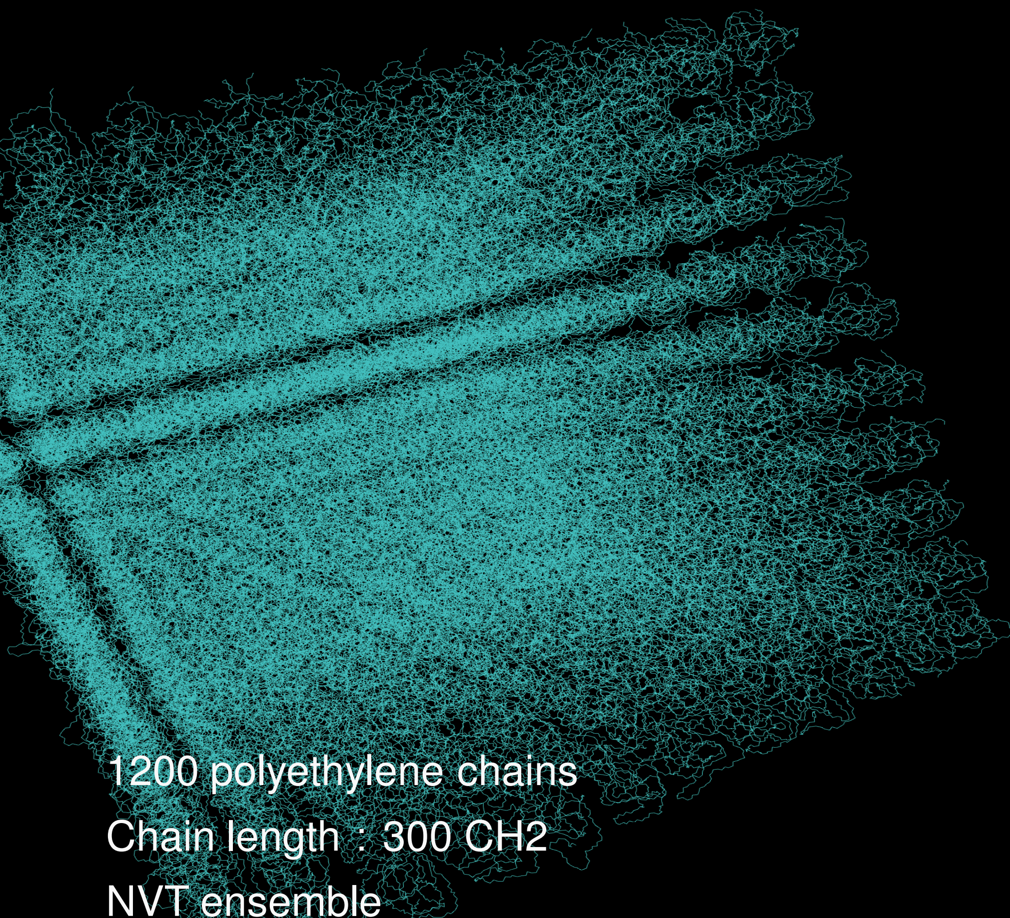








Biochemistry:



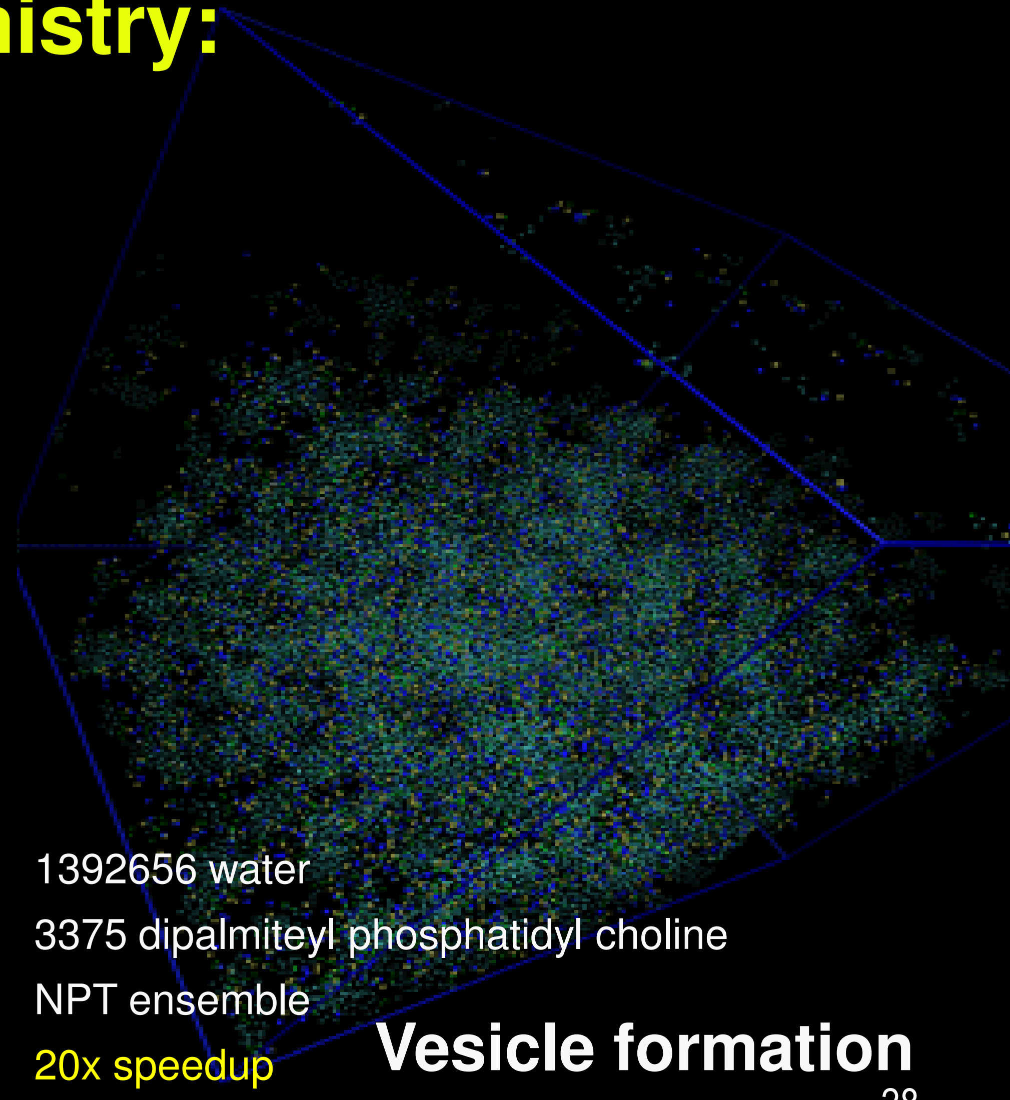
1200 polyethylene chains

Chain length : 300 CH2

NVT ensemble

30x speedup

Polymer dynamics



1392656 water

3375 dipalmiteyl phosphatidyl choline

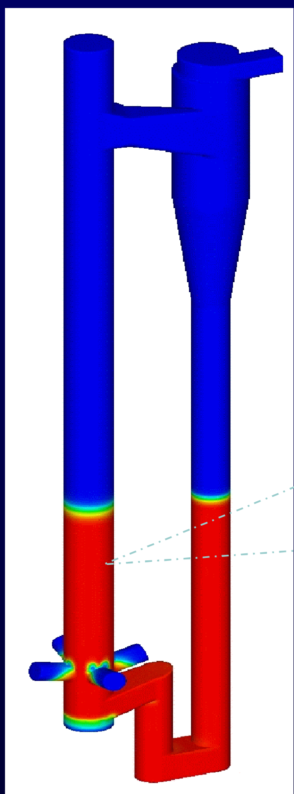
NPT ensemble

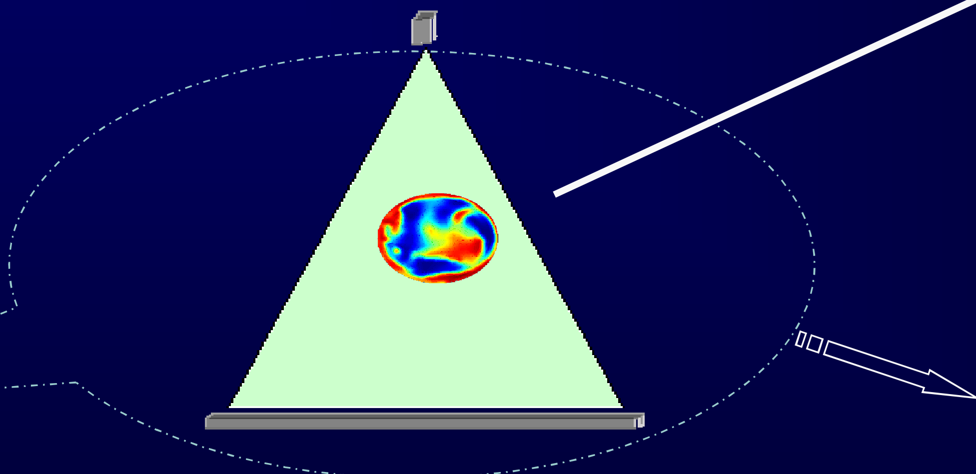
20x speedup

Vesicle formation

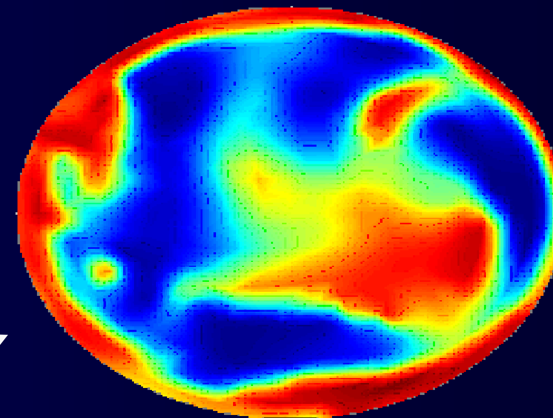
Data processing:

Image reconstruction for industrial CT

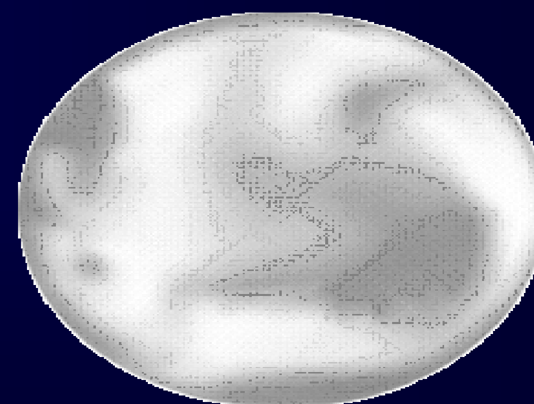




Scanning



realtime



off-line

>80x speedup

Prospect of virtual process engineering

hardware + software → application

CPU

CPU+GPU

macro

meso

micro

CPU+XPU+GPU

macro meso micro

average

multi-scale discrete

pre-/post-processing

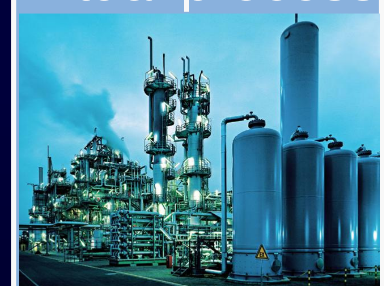
engineering design

simulator

CAD

realtime

virtual process



Summary

- Similarity between problem, software and hardware is key to real HPC.

- Multi-scale discrete simulation is natural and advantageous way for the simulation of a wide variety of complex systems.

- GPU computing provides an effective way to realize multi-scale discrete simulation with commercial components.

Thank you

for your attention !

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(to be updated)

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