JIAN ZHANG

Dr. Jian Zhang received the PhD in applied mathematics at the University of Minnesota in 2005. From June 2005 to June 2009, he was a postdoc in the Pennsylvania State University working on scientific computing and modeling. He is currently a research scientist at the Computer Network Information Center of the Chinese Academy of Sciences. His research interests include scientific computing and high performance computing.

Large-scale Phase Field Simulation for Coarsening Dynamics Based on Cahn-Hilliard Equation with Degenerated Mobility

Large scale phasefield simulation for coarsening dynamics based on the Cahn-Hilliard equation with degenerated mobility

Jian Zhang

Computer Nework Information Center(CNIC), CAS

Chunbao Zhou(CNIC), Yangang Wang(CNIC), Xuebin Chi(CNIC),

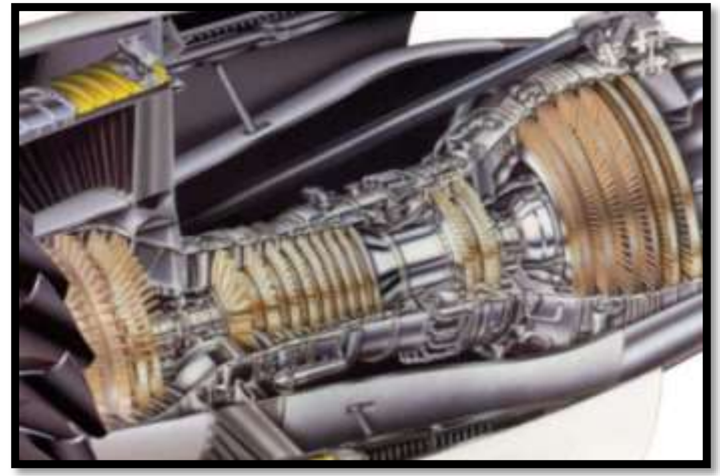
Lili Ju(USC), Qiang Du(Columbia) , Dongsheng Xu(IMRCAS)

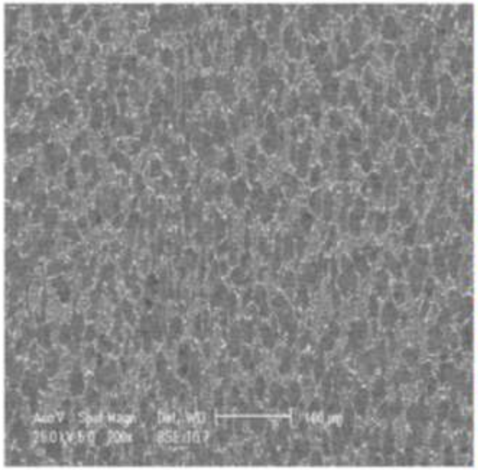
Coarsening

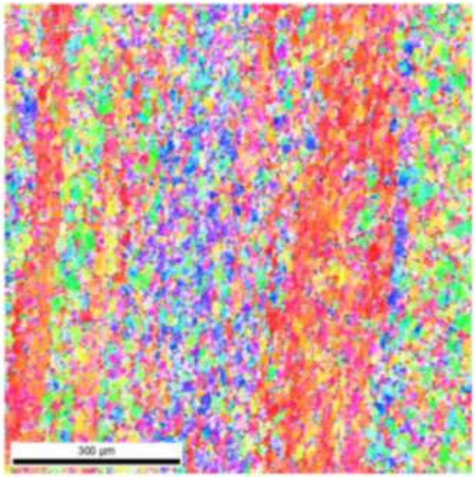
changes in spatial scales over time associated with the mesoscale morphological patterns (micro-structures).

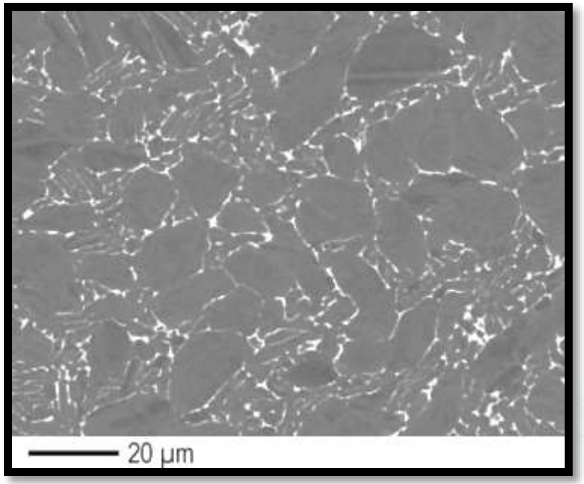
critical role in determining many material properties

strenth, hardness, fatigue, ...









Phase Field Model

Diffuse interface model, leads to a set of Partial Differential Equations

non-conserved field variable(phase) Allen-Cahn, TDGL equation,
2nd order diffusion-reaction equation

$$\frac{\partial \eta_p(r,t)}{\partial t} = -L \frac{\delta F}{\delta \eta_p(r,t)} + \xi_p(r,t);$$

conserved field variable(composition) Cahn-Hilliard equation,
4th order nonlinear diffusion

$$\frac{\partial c(r,t)}{\partial t} = \nabla \bullet [M \nabla \frac{\delta F}{\delta c(r,t)}] + \zeta(r,t).$$

Computationally challenging:

various spacial and temporal scale

stiffness and strong nonlinear effects

Explicit Finite Difference

$$u_t = Lu + N(u,t)$$

stencil computation

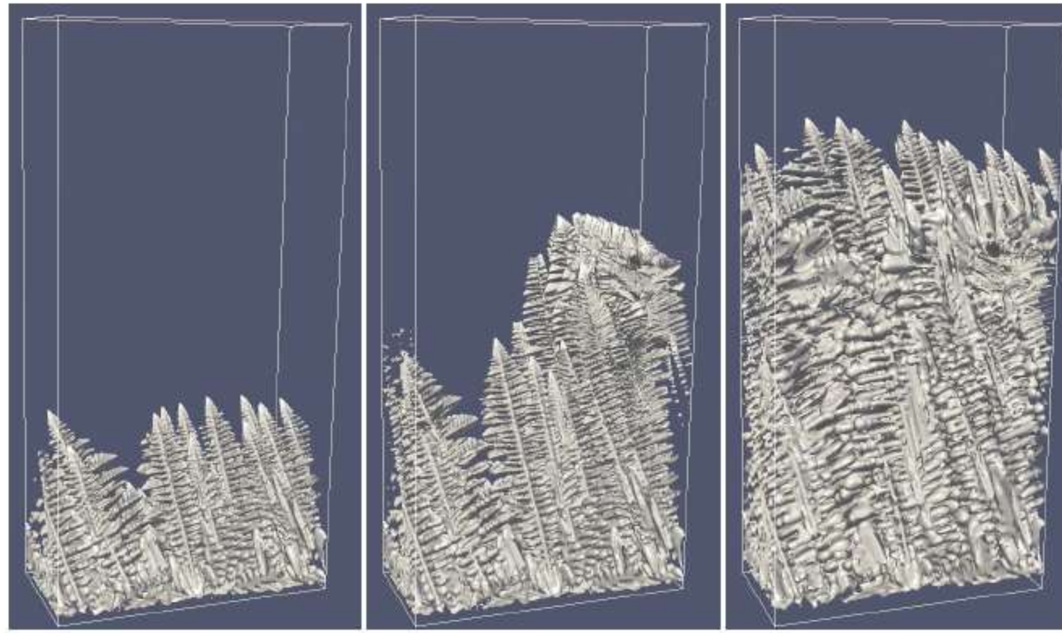
$$u^{n+1} = u^n + \Delta t[Lu^n + N(u^n, t^n)]$$

$$\frac{1}{(\Delta x)^r}$$

stability resriction: $\Delta t \propto (\Delta x)^r$

Large scale long time simulation

Allen-Cahn Equ. (r=2): YES!
Cahn-Hilliard Equ. (r=4): NO!

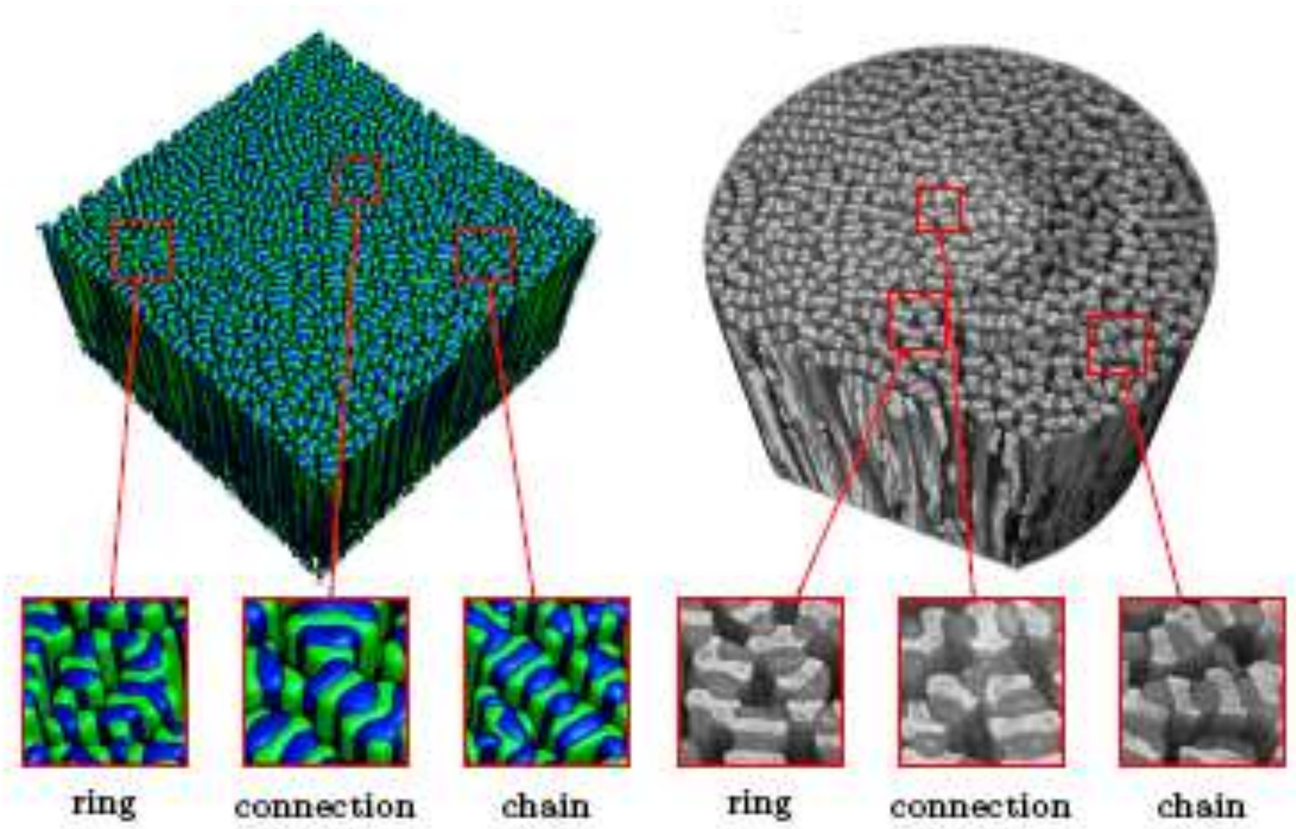


Takashi Shimokawabe et. al. SC2011

Gordon Bell Prize, Scalability

binary dendritic growth

Explicit Finite Difference



Martin Bauer et. al. SC2015

directional solidification,
Allen-Cahn type equation, omitting the coarsening effect

Implicit Finite Difference

$$u_t = Lu + N(u,t)$$

$$u^{n+1} = u^n + \Delta t[Lu^{n+1} + N(u^n, t^n)]$$

$$\frac{1}{(\Delta x)^r}$$

stability issue resolved at the prize of solving
large scale sparse linear/nonlinear systems at each time step

$$u^{n+1} = u^n + \Delta t[Lu^{n+1} + N_1(u^{n+1}, t^{n+1})] + N_2(u^n, t^n)]$$

operator spiltting,
introducing 1st order splitting error

Exponential Time Differencing

$$u_t = Lu + N(u, t).$$

$$u(t_{n+1}) = e^{L\Delta t} u(t_n) + e^{L\Delta t} \int_0^{\Delta t} e^{-Ls} N(u(t_n + s), t_n + s) ds.$$

exact integration， no stability issue

$$U = \begin{pmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{pmatrix}_{N_x \times N_y \times N_z} \qquad e^{L\Delta t} = \begin{pmatrix} \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \end{pmatrix}_{(N_x \times N_y \times N_z) \times (N_x \times N_y \times N_z)}$$

however, dense exponential matrices

$1{,}000^3$ simulation,（10^9） grid points

$\Longrightarrow$ Exa（10^{18}）strorage and computation

Compact representation of FD discretization

$$u_t = D\Delta u + F(u,t)$$

$$A = \frac{D}{h_x^2}\begin{pmatrix} -\frac{2}{3} & \frac{2}{3} & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & \frac{2}{3} & -\frac{2}{3} \end{pmatrix}_{N_x \times N_x}$$

$$B = \frac{D}{h_y^2}\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -2 & 1 \\ 1 & 0 & \cdots & 0 & 1 & -2 \end{pmatrix}_{(N_y+1)\times(N_y+1)}$$

$$U = \begin{pmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,N_y} & u_{1,N_y+1} \\ u_{2,1} & u_{2,2} & \cdots & u_{2,N_y} & u_{2,N_y+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{N_x,1} & u_{N_x,2} & \cdots & u_{N_x,N_y} & u_{N_x,N_{y+1}} \end{pmatrix}_{N_x \times (N_y+1)}$$

$$\frac{dU}{dt} = AU + UB + F.$$

$$e^{A\Delta t} = \begin{pmatrix} \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \end{pmatrix}_{N_x \times N_x}$$

$1{,}000^3$ grid points ⇒

Giga（10^9）strorage and
Tera（10^{12}）computation

Linear operator splitting

$$u_t = Lu + N(u,t)$$

$$u_t = Lu \pm \tilde{L}u \mp \tilde{L}u + N(u,t)$$

Exact integration

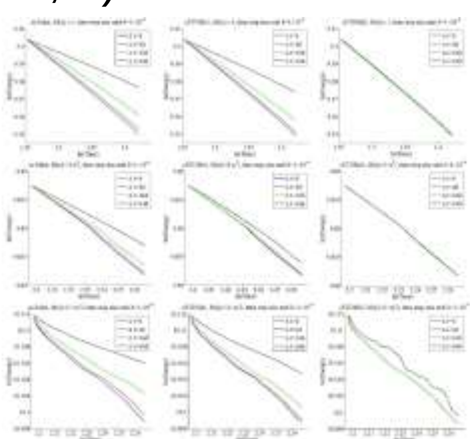
polynomial approximation

High order in nature

Important for effective simulation of coarsening process, time step size 10-100 times larger than the 1st order implict FD schemes (CMS 2015, JSC 2015,...)

Table 1
Constant mobility $M(u) \equiv 1$: numerical errors and temporal convergence rates with periodic BC.

Δt	6.4×10^{-3}	3.2×10^{-3}	1.6×10^{-3}	8×10^{-4}	4×10^{-4}	2×10^{-4}	1×10^{-4}
ss-Euler							
Rela. ener. error	2.828E−2	1.945E−2	1.217E−2	7.094E−3	3.949E−3	2.138E−3	1.135E−3
Conv. rate	–	0.54	0.68	0.78	0.85	0.89	0.91
Rela. L^2 error	1.533E−1	1.128E−1	7.434E−2	4.456E−2	2.510E−2	1.366E−2	7.288E−3
Conv. rate	–	0.44	0.602	0.74	0.83	0.88	0.91
cETDMs1							
Rela. ener. error	2.548E−2	1.631E−2	9.325E−3	4.949E−3	2.528E−3	1.271E−3	6.369E−4
Conv. rate	–	0.64	0.81	0.91	0.97	0.99	1.00
Rela. L^2 error	1.414E−1	9.693E−2	5.800E−2	3.139E−2	1.615E−2	8.165E−3	4.109E−3
Conv. rate	–	0.55	0.74	0.89	0.96	0.98	0.99
cETDMs2							
Rela. ener. error	8.453E−4	2.370E−4	6.366E−5	1.647E−5	4.233E−6	1.089E−6	2.738E−7
Conv. rate	–	1.84	1.90	1.95	1.96	1.96	1.99
Rela. L^2 error	6.011E−3	1.921E−3	5.656E−4	1.498E−4	3.766E−5	9.366E−6	2.286E−6
Conv. rate	–	1.65	1.76	1.92	1.99	2.01	2.03



ScETD method

cETD: Stable, high order accurate schemes for phase field equations.

compact representation of finite difference discretization
+ Exponential Time Differencing + linear operator splitting

Essentially explicit

- no need to slove linear/nonlinear systems

accurate large time step

- time stepsize 10-100 times larger than 1st order implicit schemes

compute intensive

- explore the computing power of modern hardware

ScETD: Scalable cETD with localized exponential integraion and subdomian coupling

explicit cETD as subdomian solver with explicit inner boundary conditions provided by adjacent subdmains.

Implimentation on Sunway TaihuLight

1 core group handles 1 subdomain:

Exponential integration of solution variables and B.C.'s
- tensor dot production DGEMM
- tensor transposition CPE's via DMA

Nonlinear terms in equation and B.C.'s
- pointwise and stencil computation CPE's via DMA

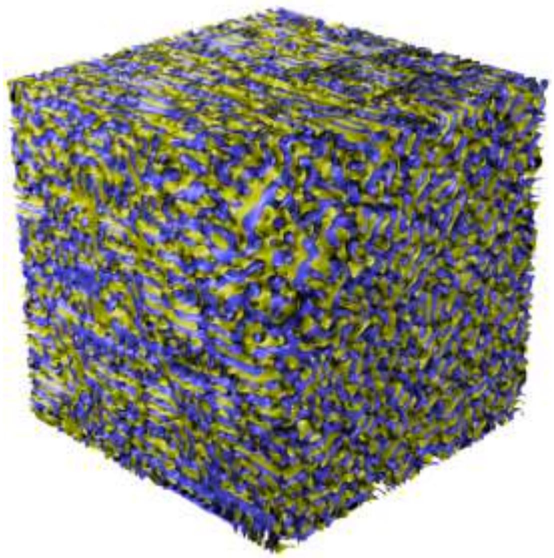
data transfer between CG's:

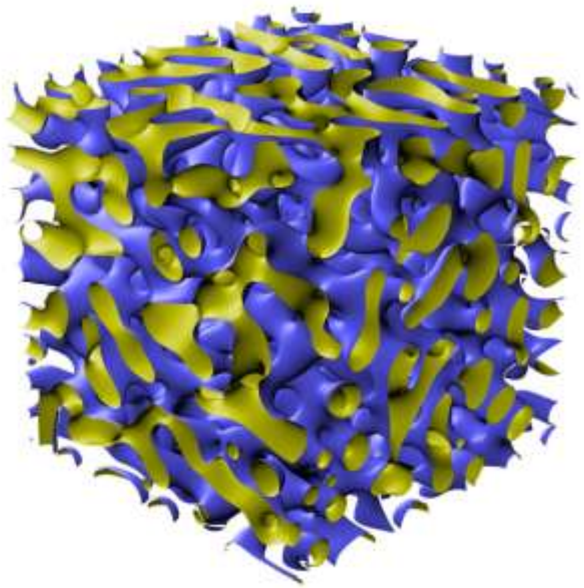
values of solution variables in the overlapping(halo) region
- packing/unpacking CPE's via DMA
- transfer MPE via MPI

I/O: MPE, asynchronous.

Coarsening dynamics simulation

Coarsening determined in both fields: CH equation with constant mobility





63 billion grid points(3972^3), 20,000 time steps, error in coarsening rate 1%.

2 million MPE and CPE cores(32,768 core groups), at 0.16sec/step, total time <1hr.

Coarsening dynamics simulation

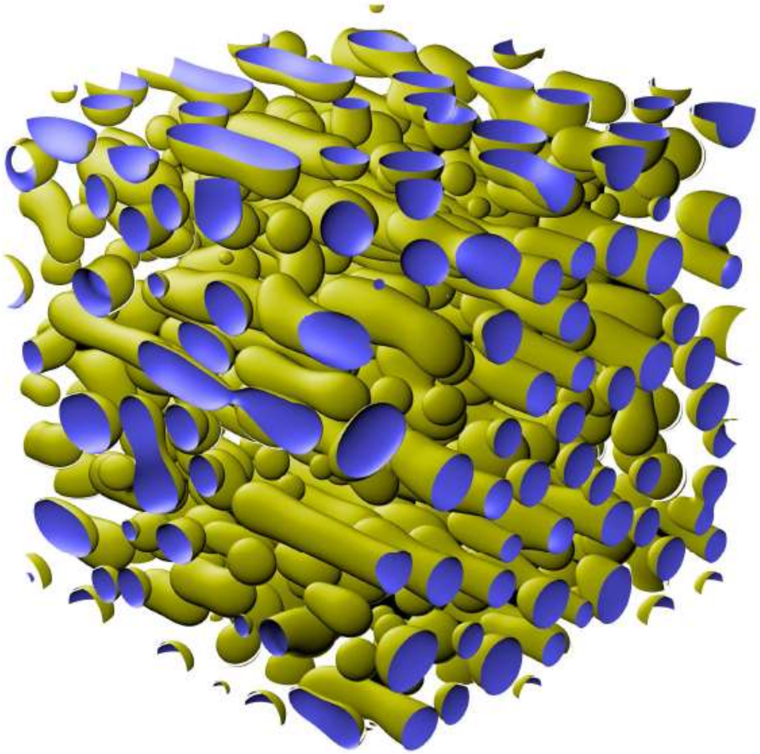
Coarsening dominented by interfacial diffusion : mobility degenerates in the two phases

slower, more nonlinear and stiff.

Different models and parameters.

63 billion grid points(3972^3),
20,000 - 100,000 time steps

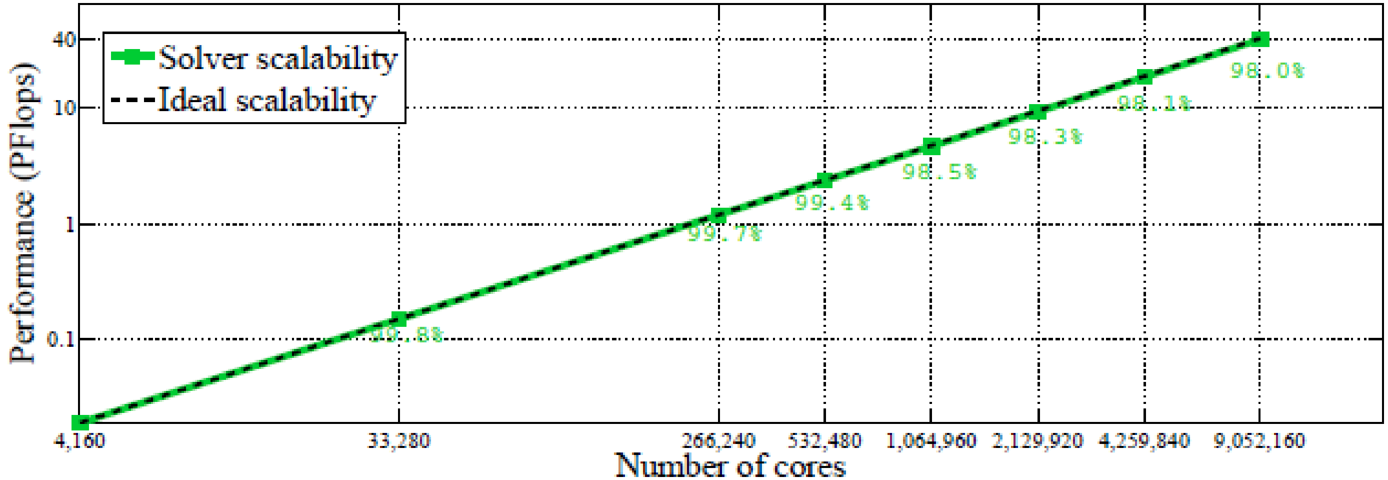
2 million MPE and CPE cores(32,768 core groups), at 0.16sec/step.



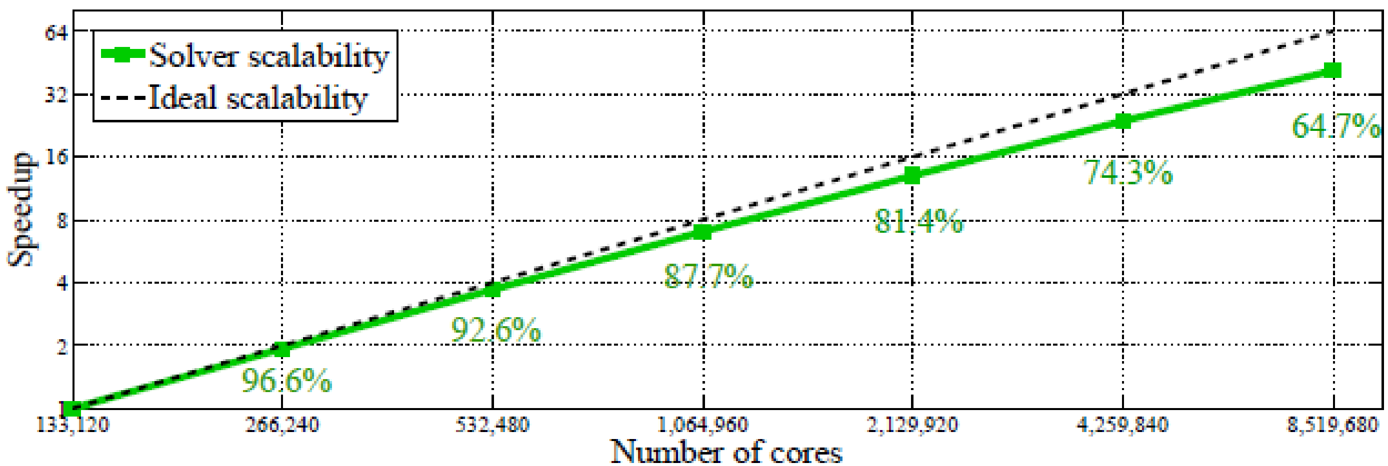
Grains in various sizes and shapes coexist, revealing transition to columnar like morphologies with unprecedented precision and details (previously reported experiments have been largely limited to resolutions with at most a handful cylinder-like structure in the computational domain).

Performance and scaling

Weak scaling, up to 18.3 trillion grid points



Strong scaling,0.27 trillion grid points.



Thanks!