Performance tests of the large scale parallel LBM-CA model of dendritic growth

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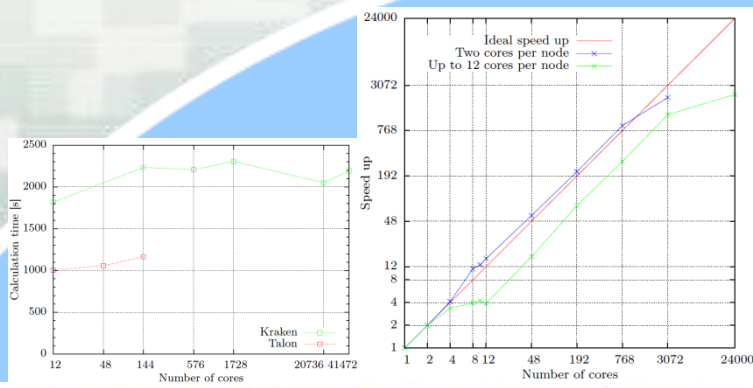

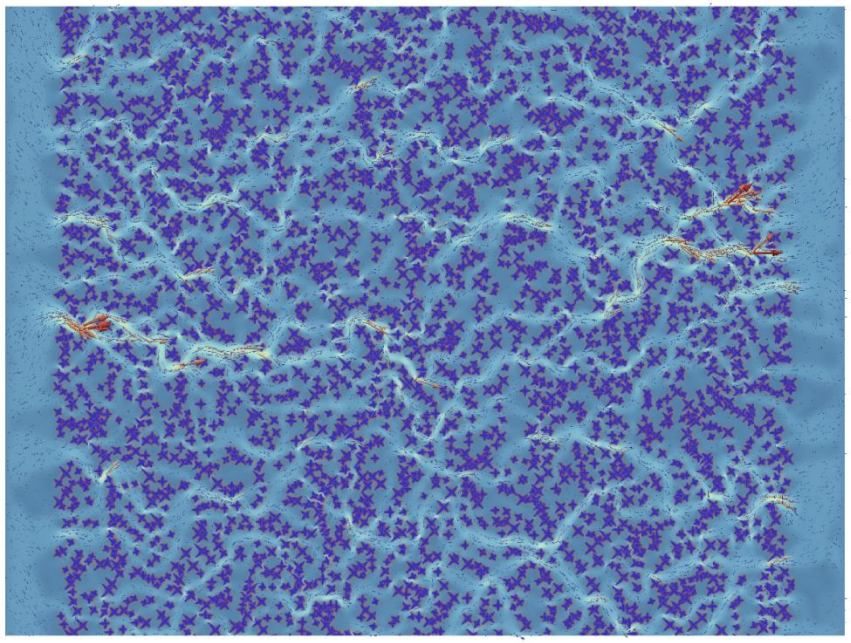

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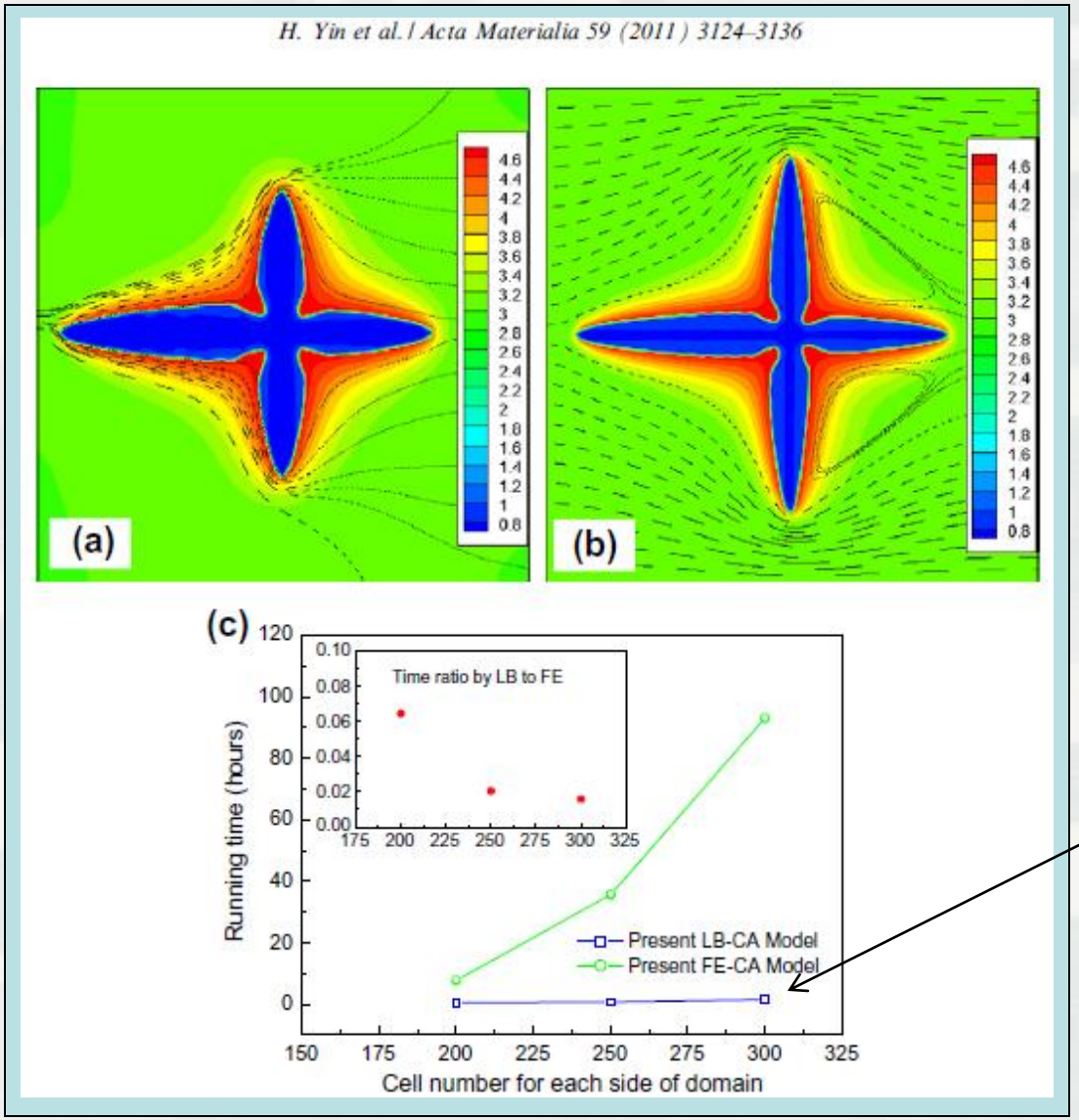
Why LBM-CA?

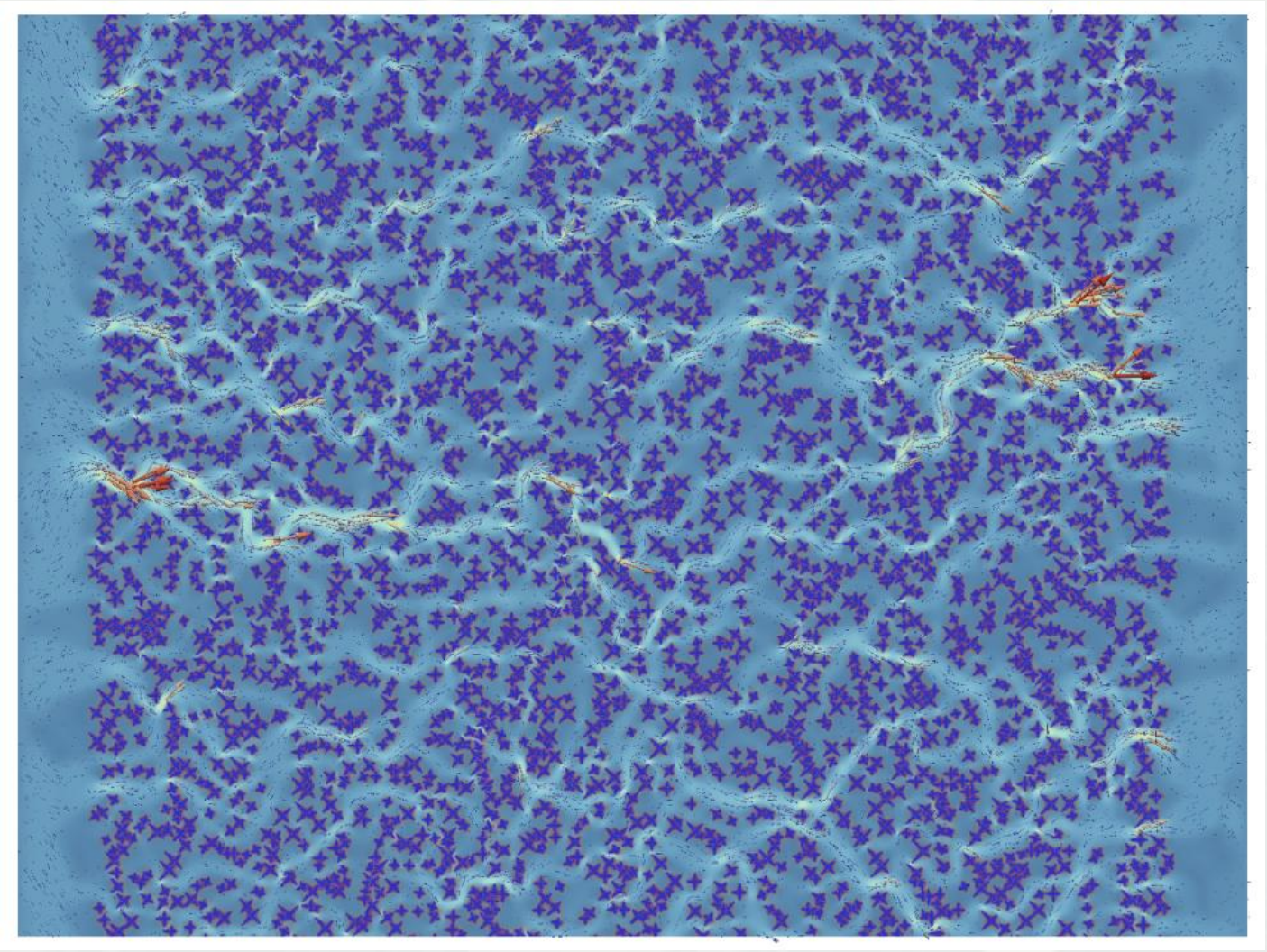


When fluid flow around solidifying dendrites is considered, lattice Boltzmann method is faster than alternatives

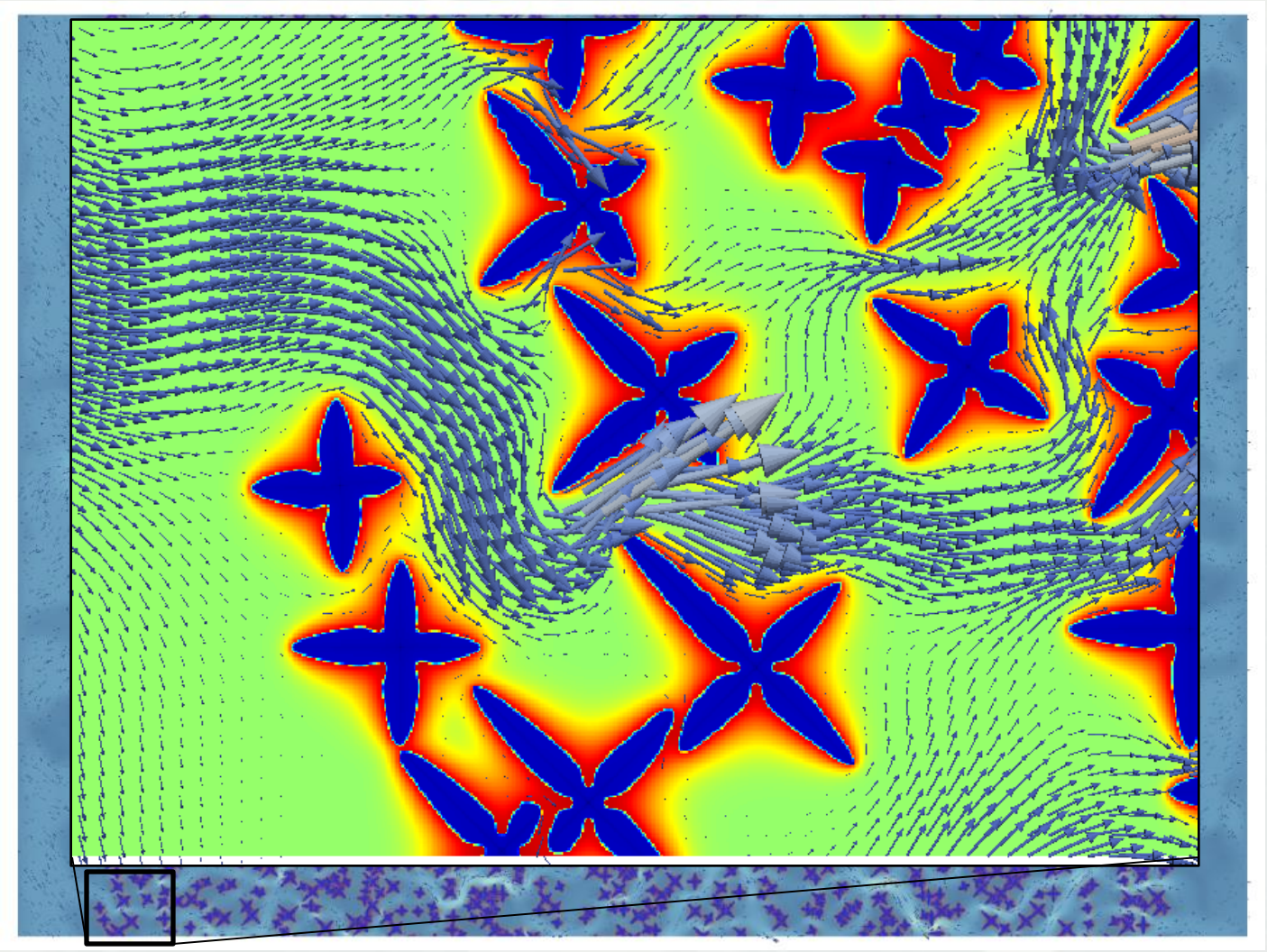
Incubation domain for parallel scaling tests

- 8000x6000 domain, chosen to fill up the memory of 1 node (12 cores) of Kraken
- Dimensions 2.4 mm x 1.8 mm, 3264 random dendrite nucleation sites
- Constant cooling rate across the whole domain, 400k time steps, periodic boundary conditions, forced melt flow through inlet (left) and outlet (right) boundaries
- Took about 10 hours on 192 cores of Talon

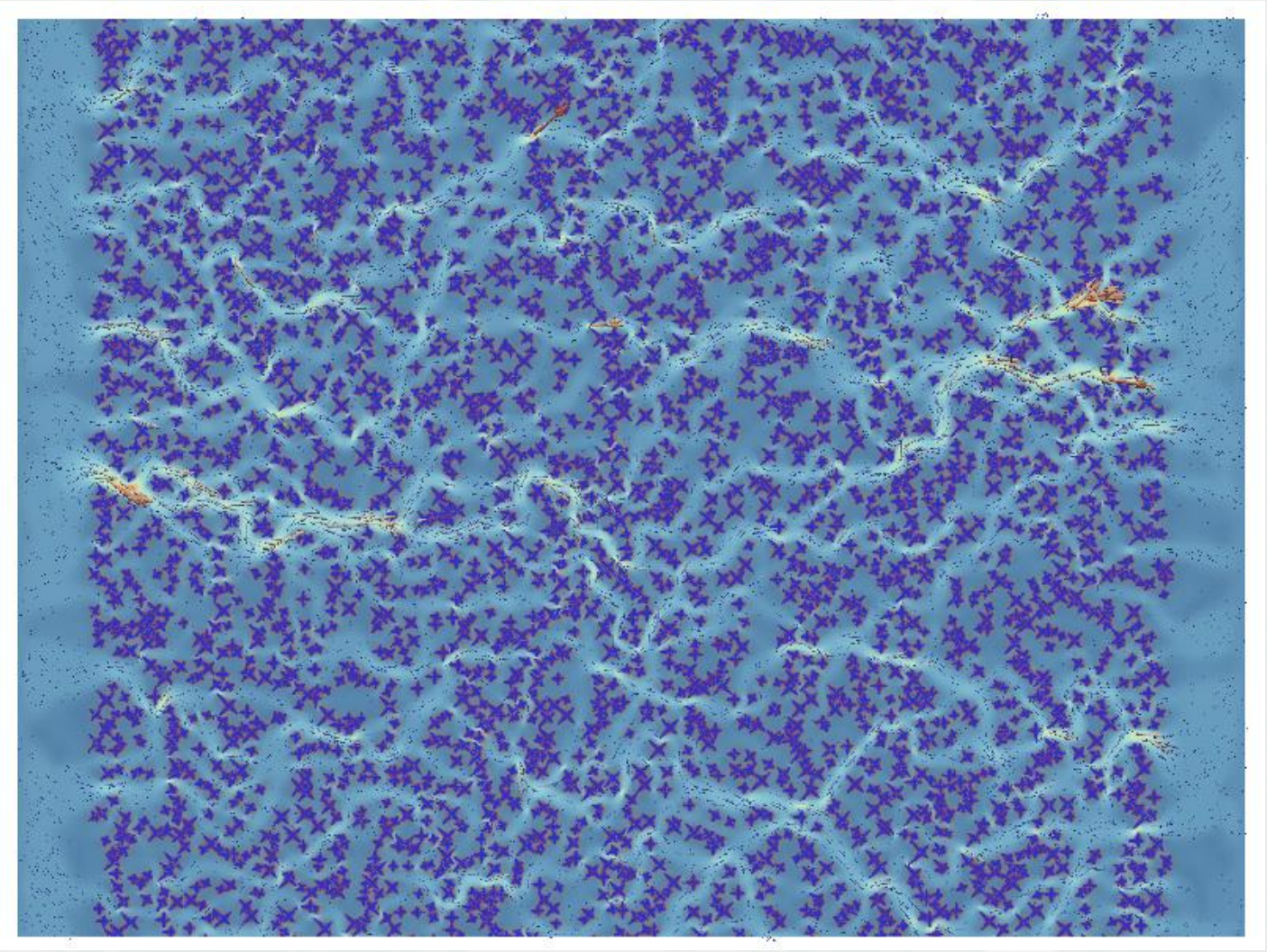
Incubation domain



Incubation domain – magnified portion



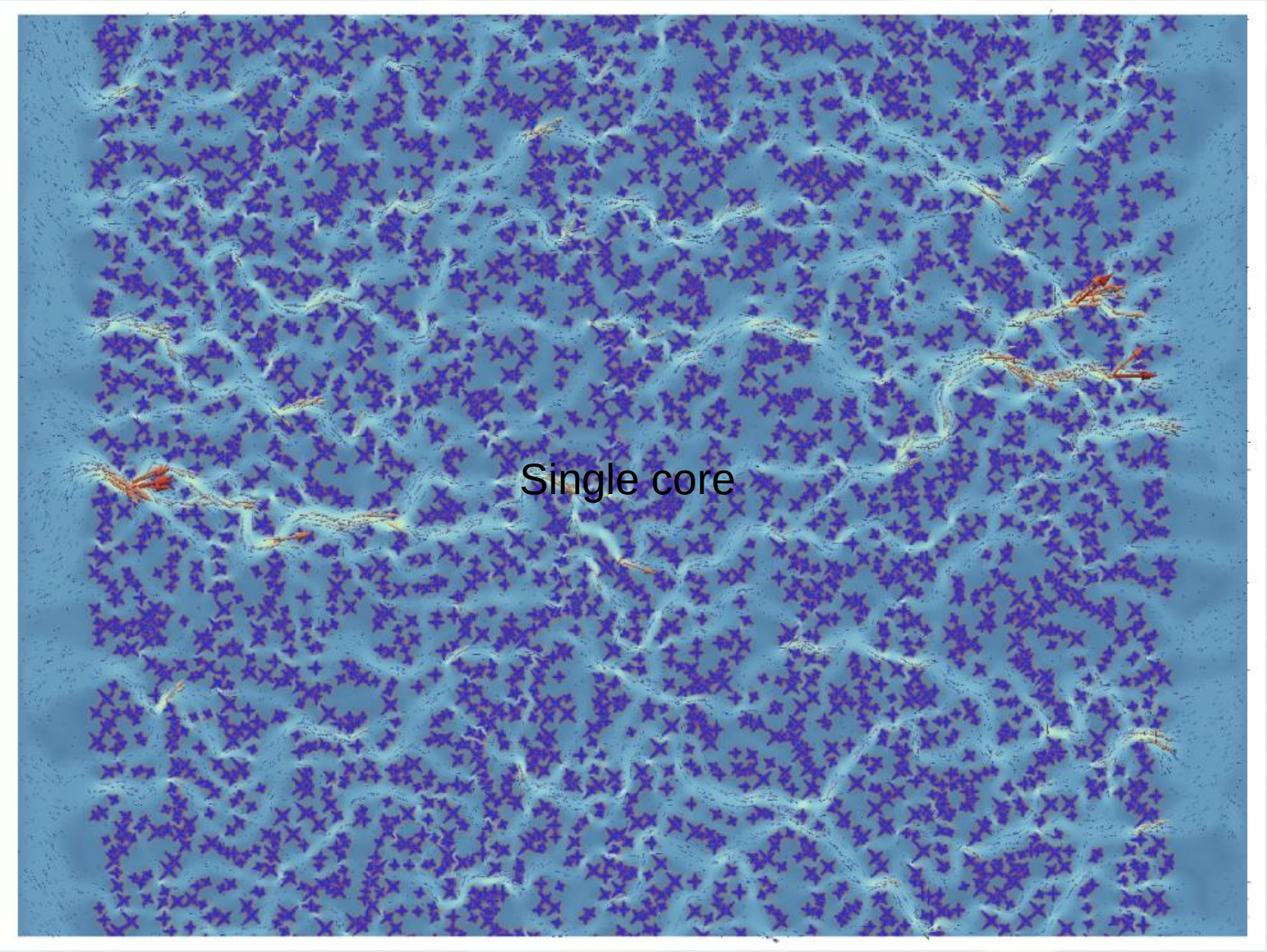
Incubation domain - animation



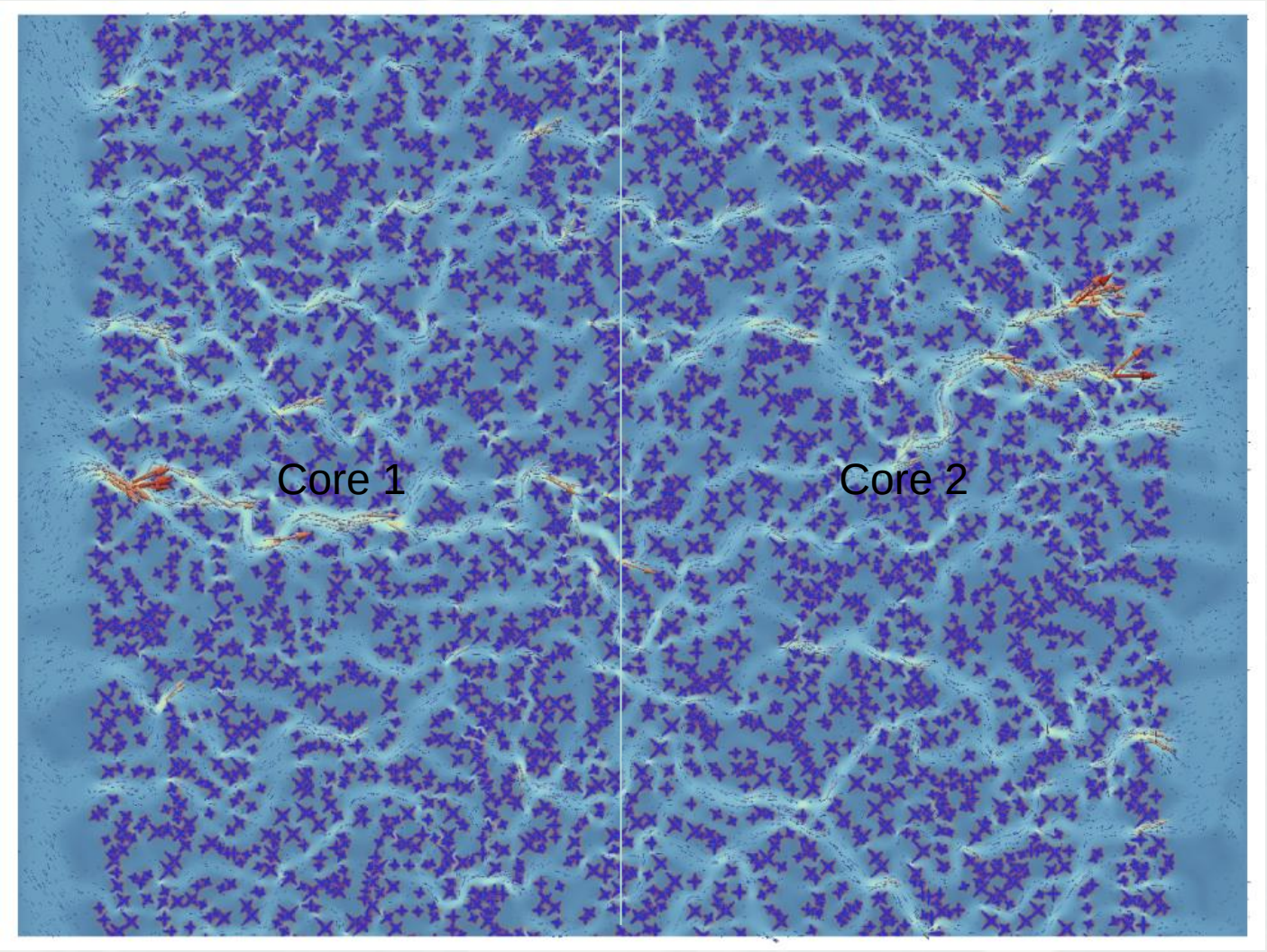
Speed up

- Speed up (strong scaling) represents how much faster a task is solved utilizing multiple cores
- Speed up tests were performed by restarting simulation from the step when the dendrites were fairly grown in the incubation domain
- Incubation domain is “split” equally between varying number of cores, then executed for 587 time steps with a flow forced at the inlet (left) and outlet (right), and with a specified cooling flow rate at all boundaries

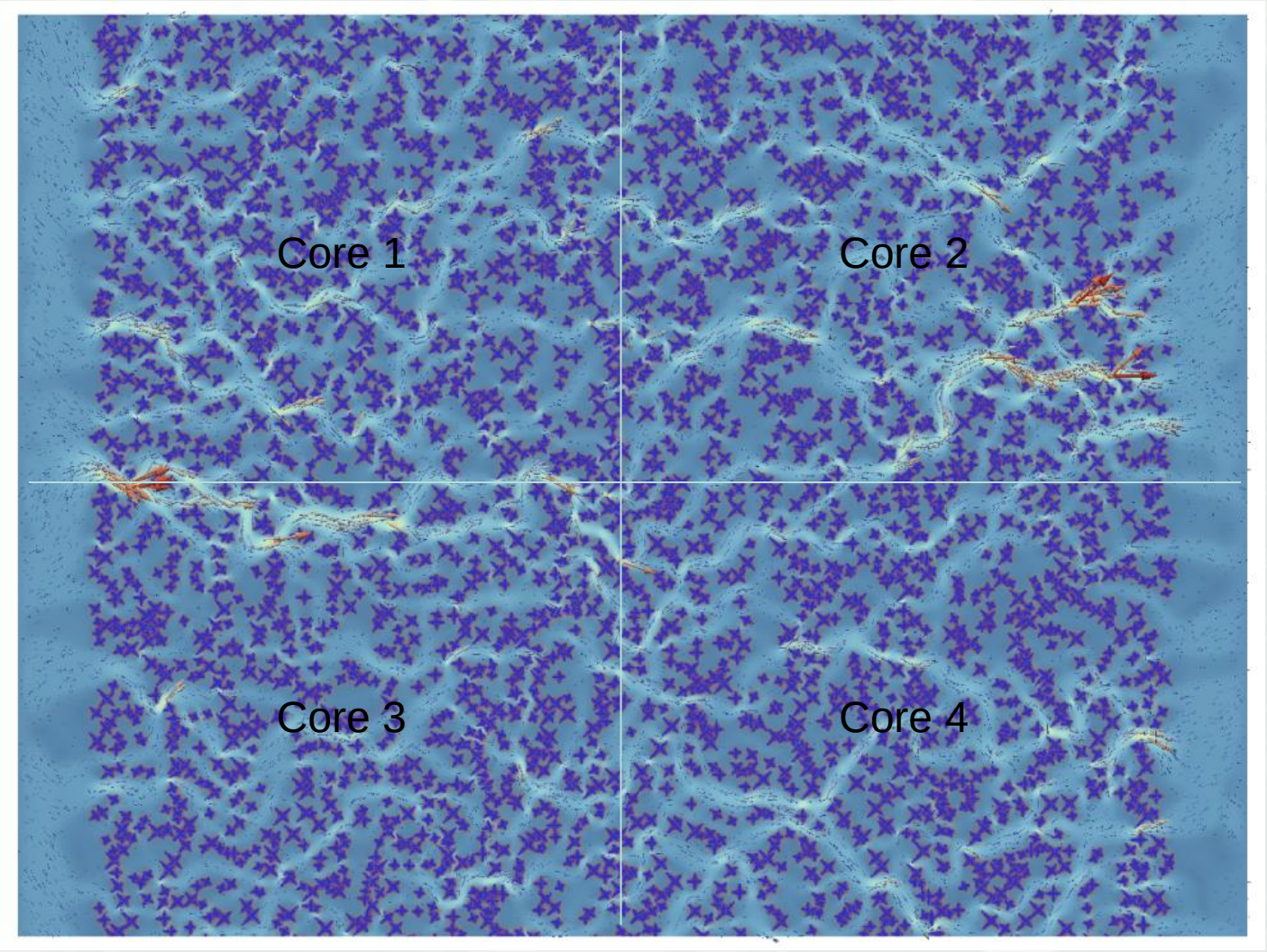
Speed up - constant task, 1 core



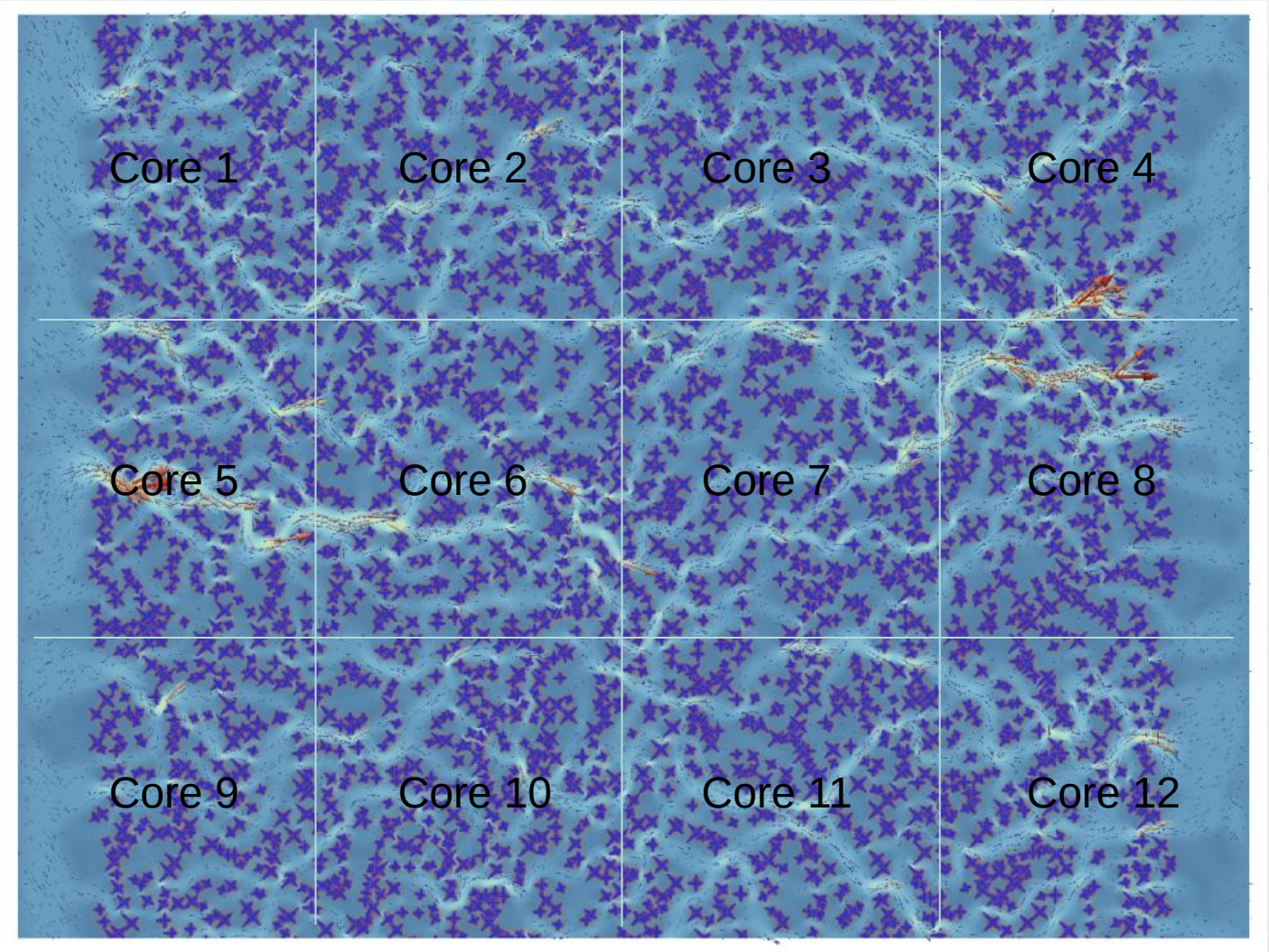
Speed up - constant task, 2 cores



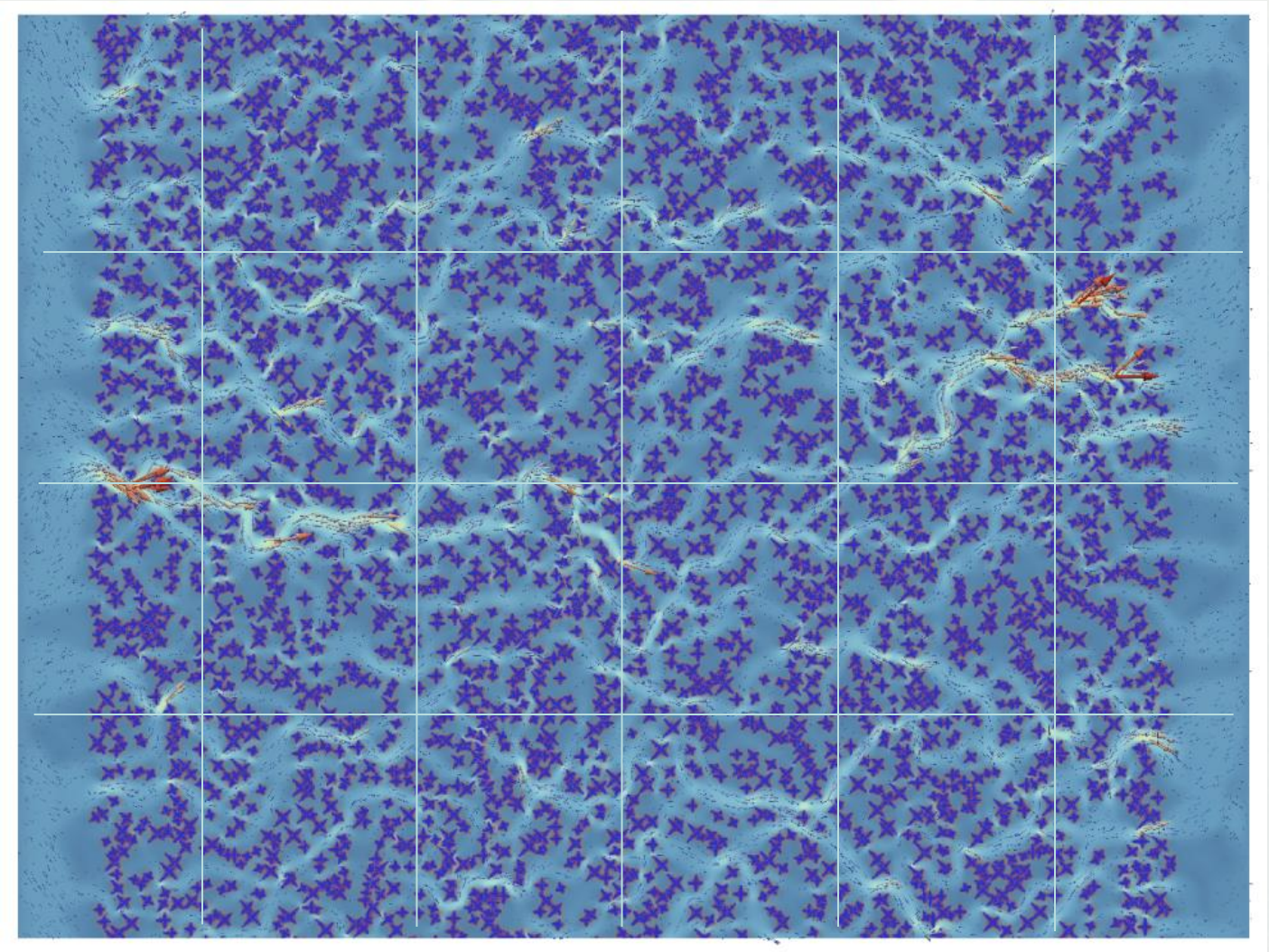
Speed up - constant task, 4 cores



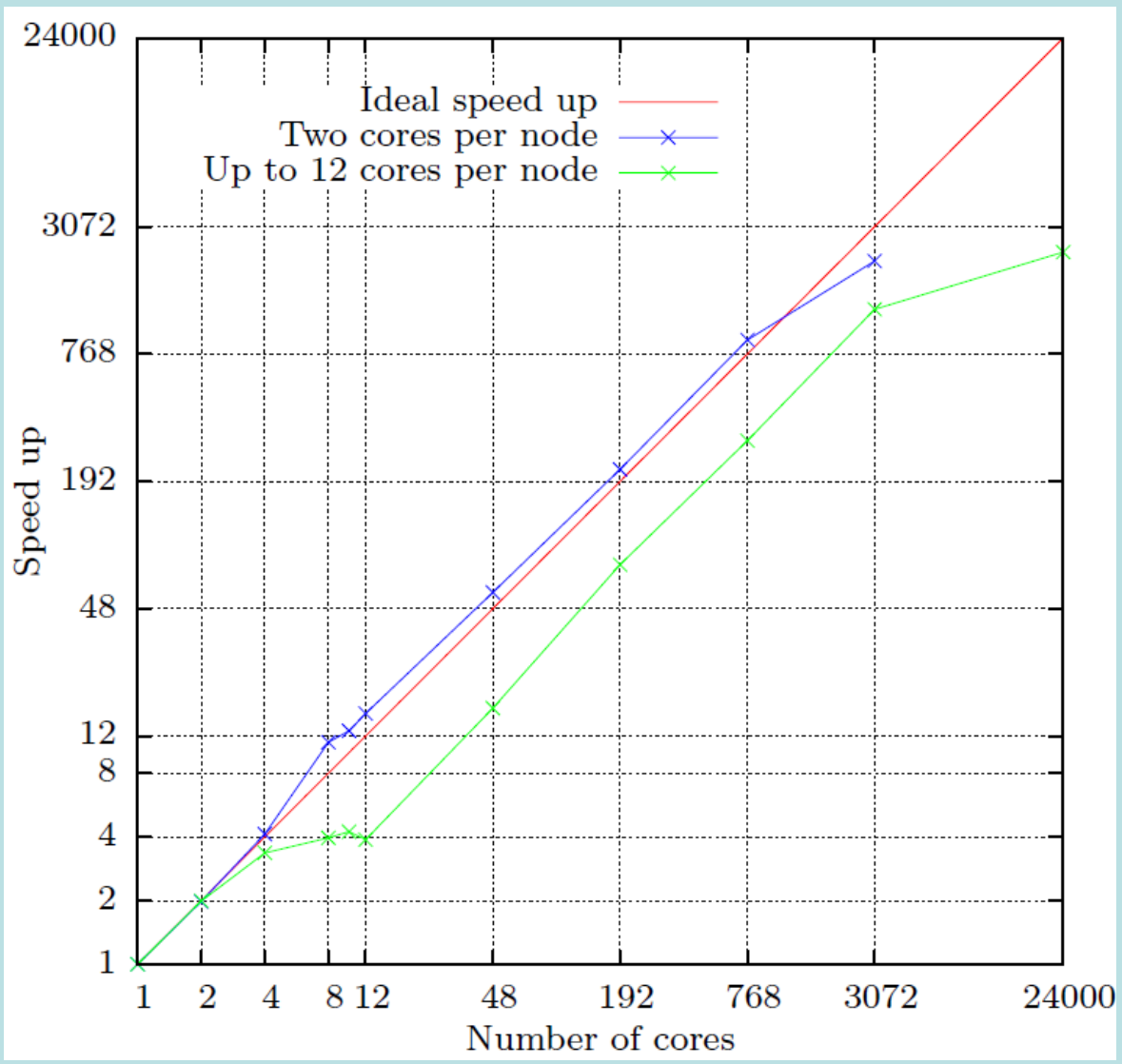
Speed up - constant task, 12 cores



Speed up - constant task, 24 cores



Speed up - results

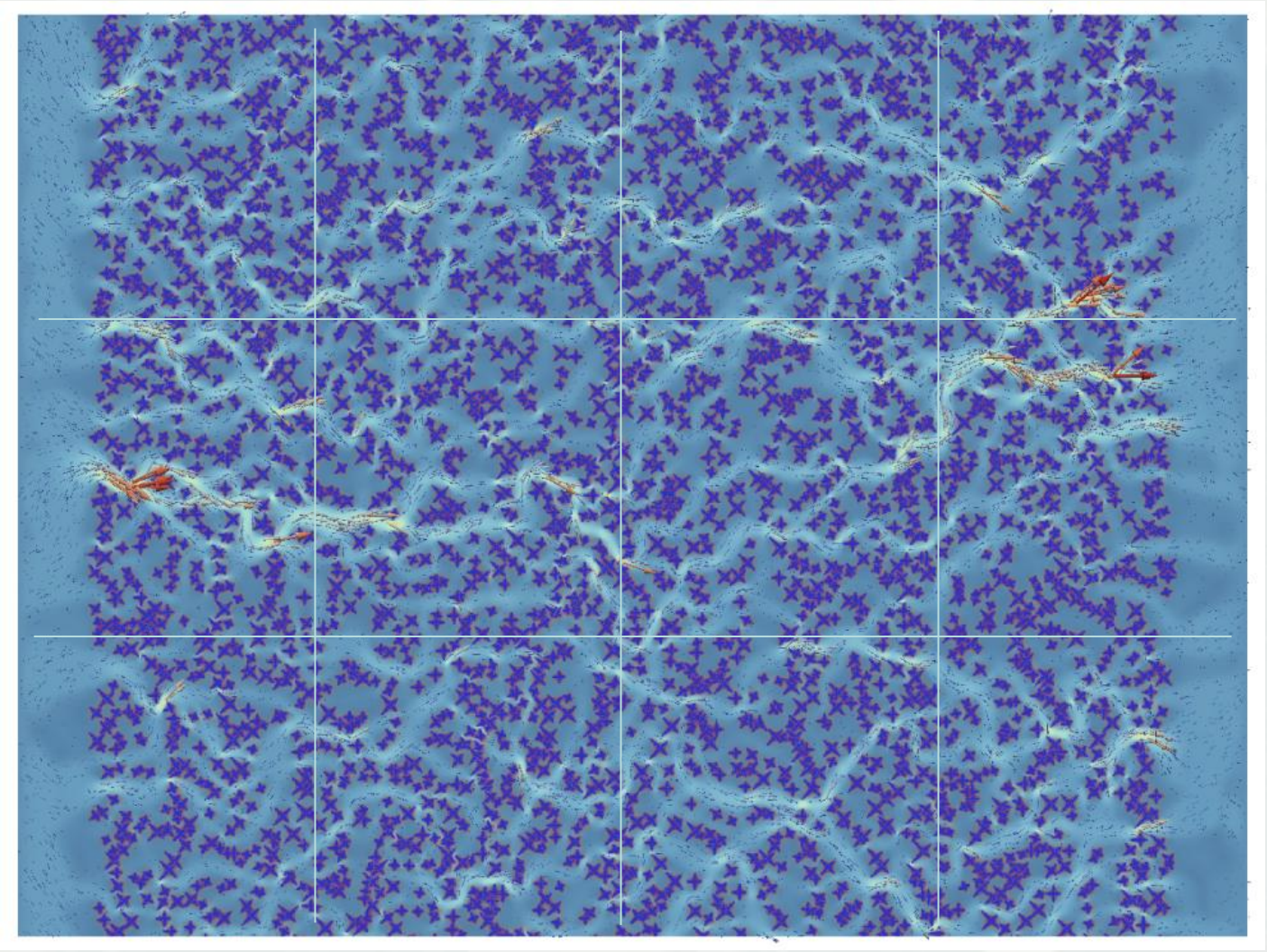


- strong scaling (speed up) near perfect up to 3072 cores
- Algorithm is memory bandwidth limited on multi-core architecture (low FLOP/byte ratio)

Scale up

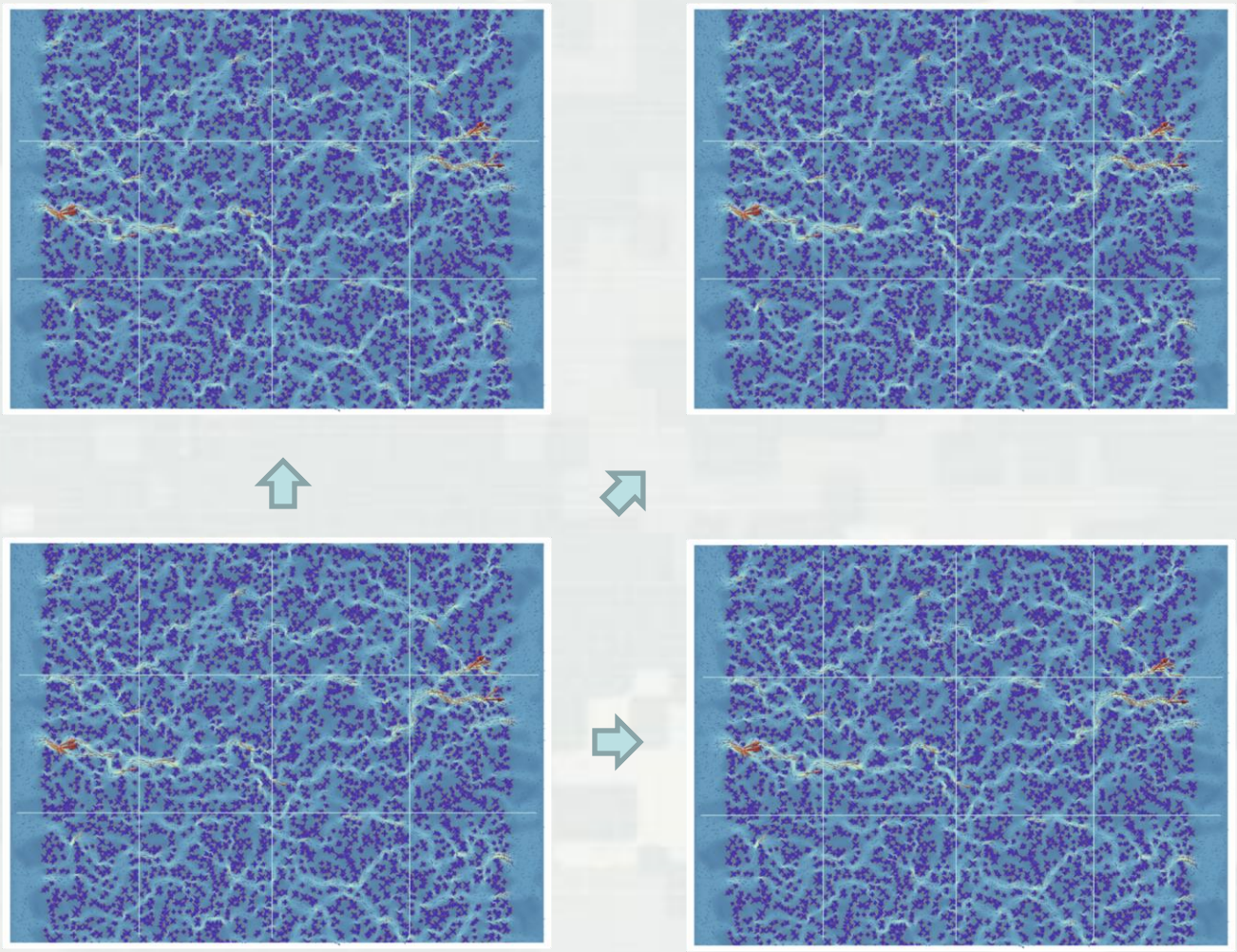
- Scale up (weak scaling) tests check if the algorithm can solve larger task when more cores are utilized without a significant performance penalty
- Scale up tests were initialized from the step when the dendrites were fairly grown in the incubation domain
- Incubated domain is “duplicated” equally onto varying number of nodes, then executed for 587 time steps with a flow forced at the inlet (left) and outlet (right), and with a specified cooling flow rate at all boundaries

Scale up - constant domain per node



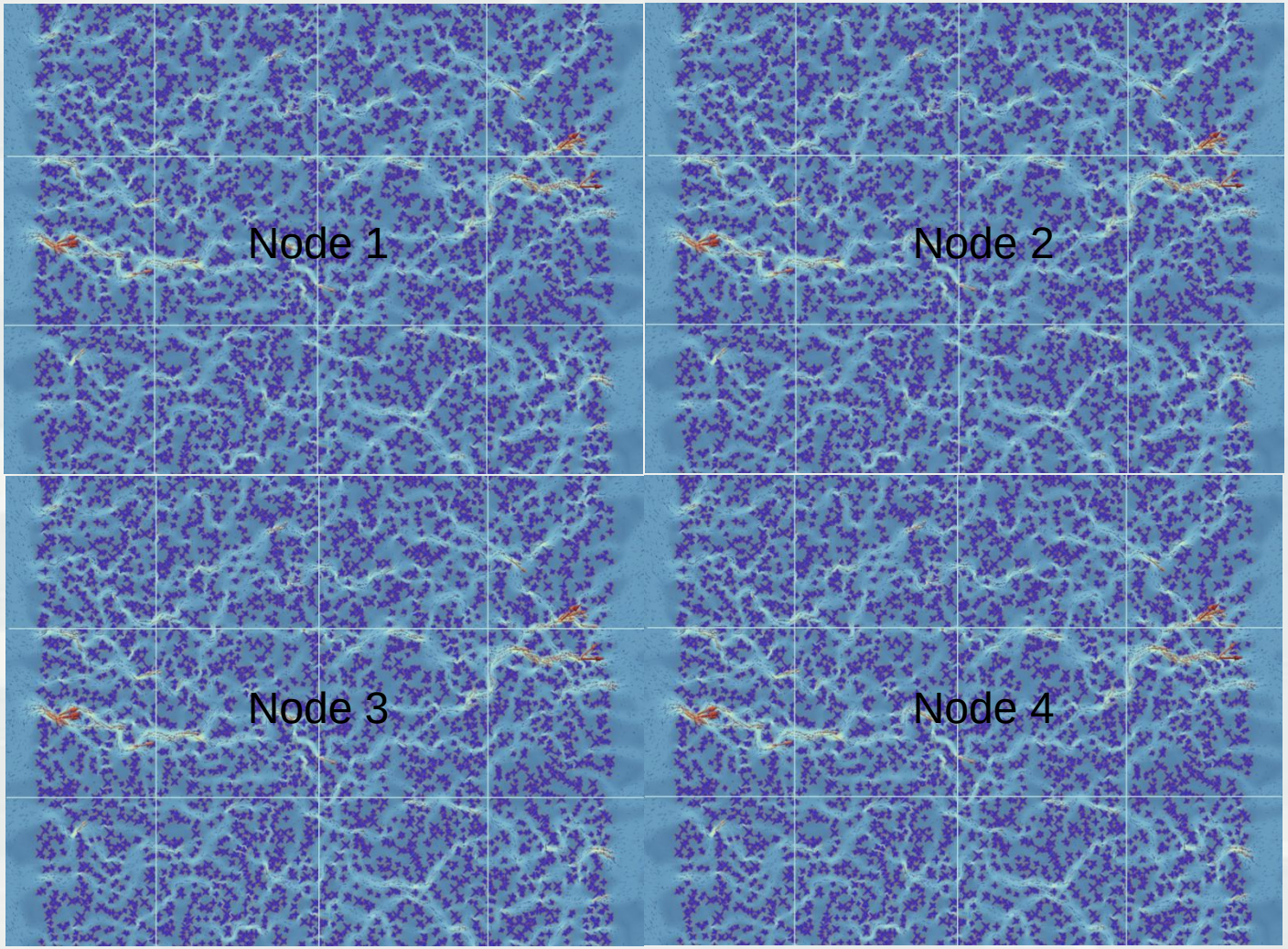
Base domain

Scale up - constant domain per node



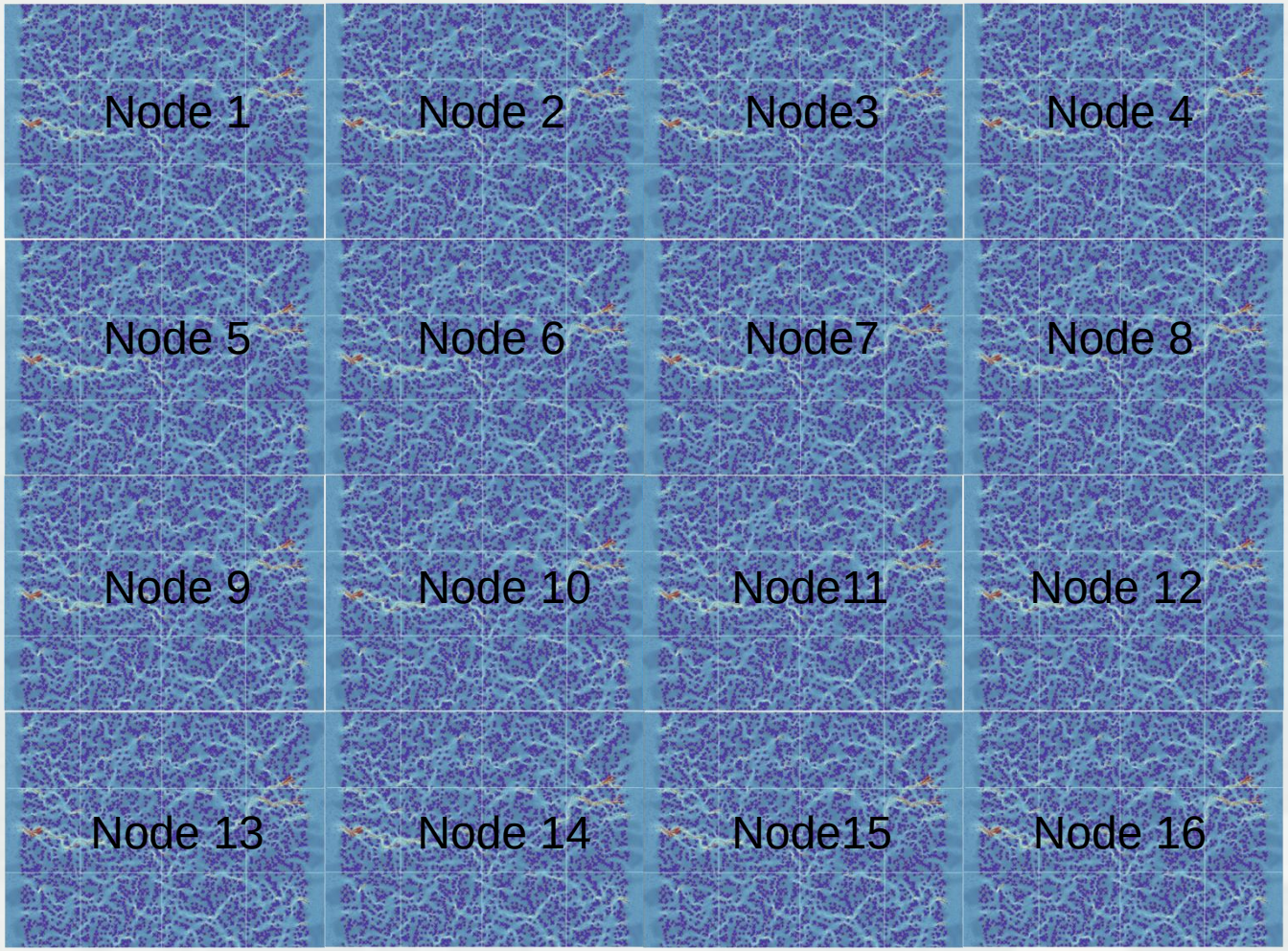
Duplication of the incubation domain onto 4 nodes

Scale up - constant domain per node



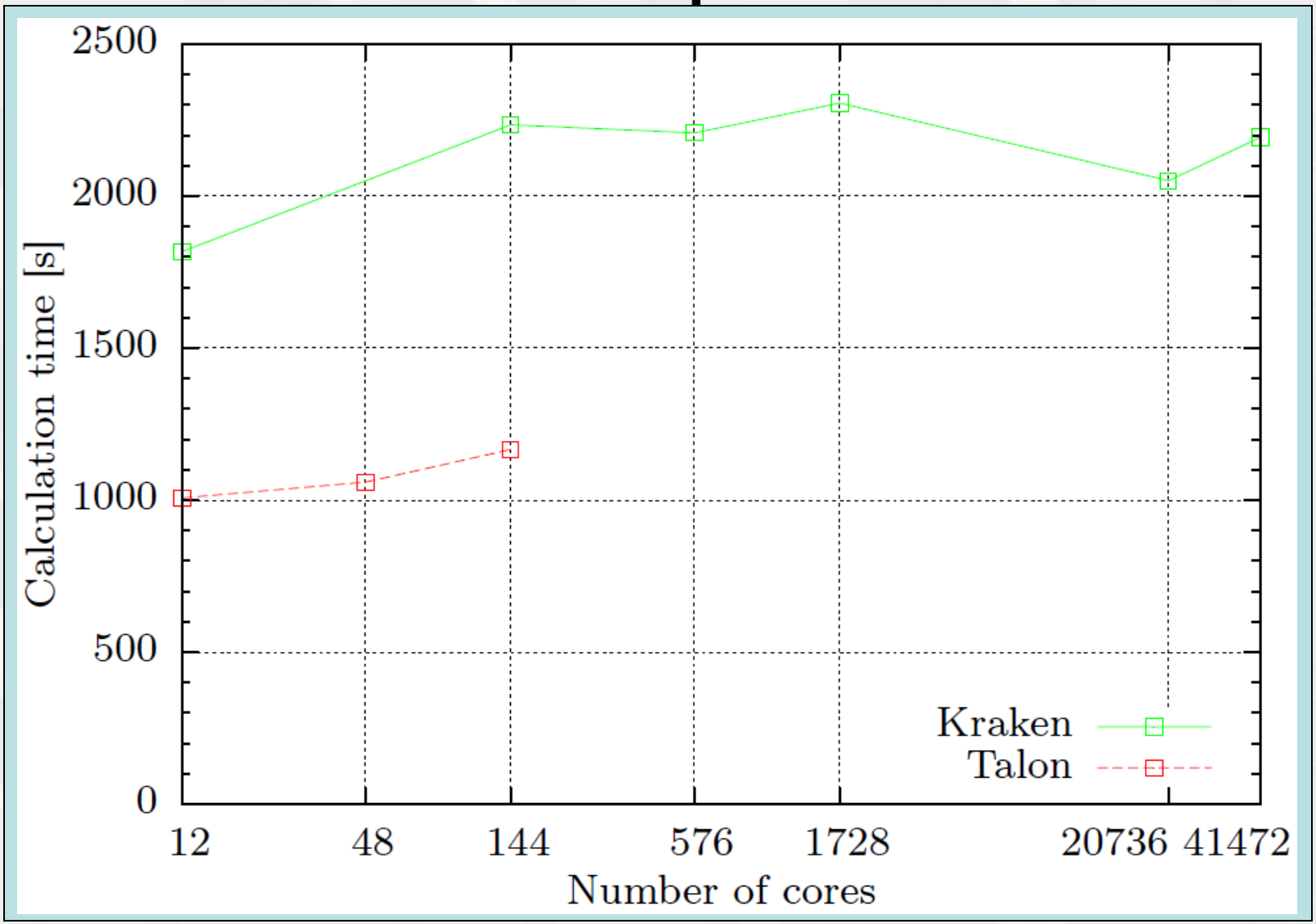
Duplication of the incubation domain onto 4 nodes

Scale up - constant domain per node



Duplication of the incubation domain onto 16 nodes

Scale up - results



Goal: constant calculation time

Scale up - results

Demonstrated nearly perfect scale up

Largest domain:

- 11 millions of dendrites (only hundreds reported before)
- solute diffusion, melt convection, and heat transport
- dimensions 17.28 cm x 8.64 cm
- over 165 billion grid nodes
- 587 time steps
- 40 minutes of simulation time
- 41472 cores of Kraken

Computational resources

Talon, MSU HPC^2:

- 3072 cores, 12 cores/node
- Intel Xeon X5660 @2.8GHz (Westmere) processors
- 24 GByte/node memory
- Voltaire quad data-rate InfiniBand (40Gb/s)
- peak performance of over 34.4 TeraFLOPS

Kraken, NICS/ORNL:

- 112,896 cores, 12 cores/node
- AMD Opteron (Istanbul) @2.6GHz (Istanbul) processors
- 16 GByte/node memory
- Cray SeaStar2+ router
- peak performance of 1.17 PetaFLOPS

XSEDE allocations

1) Simulations for 2D and 3D dendrite growth during alloy solidification:

- SDSC-GORDON 250 kSU
- NICS-KRAKEN 249 kSU
- TACC-LONESTAR 1 kSU
- ECSS

2) Large scale 3D modeling of microstructural evolution during alloy solidification

- SDSC-GORDON 500 kSU
- NICS-NAUTILUS 10 kSU

Progress on the parallelization of the 3D LBM/CA code

Already implemented

- Solute concentration and dendrite growth in parallel

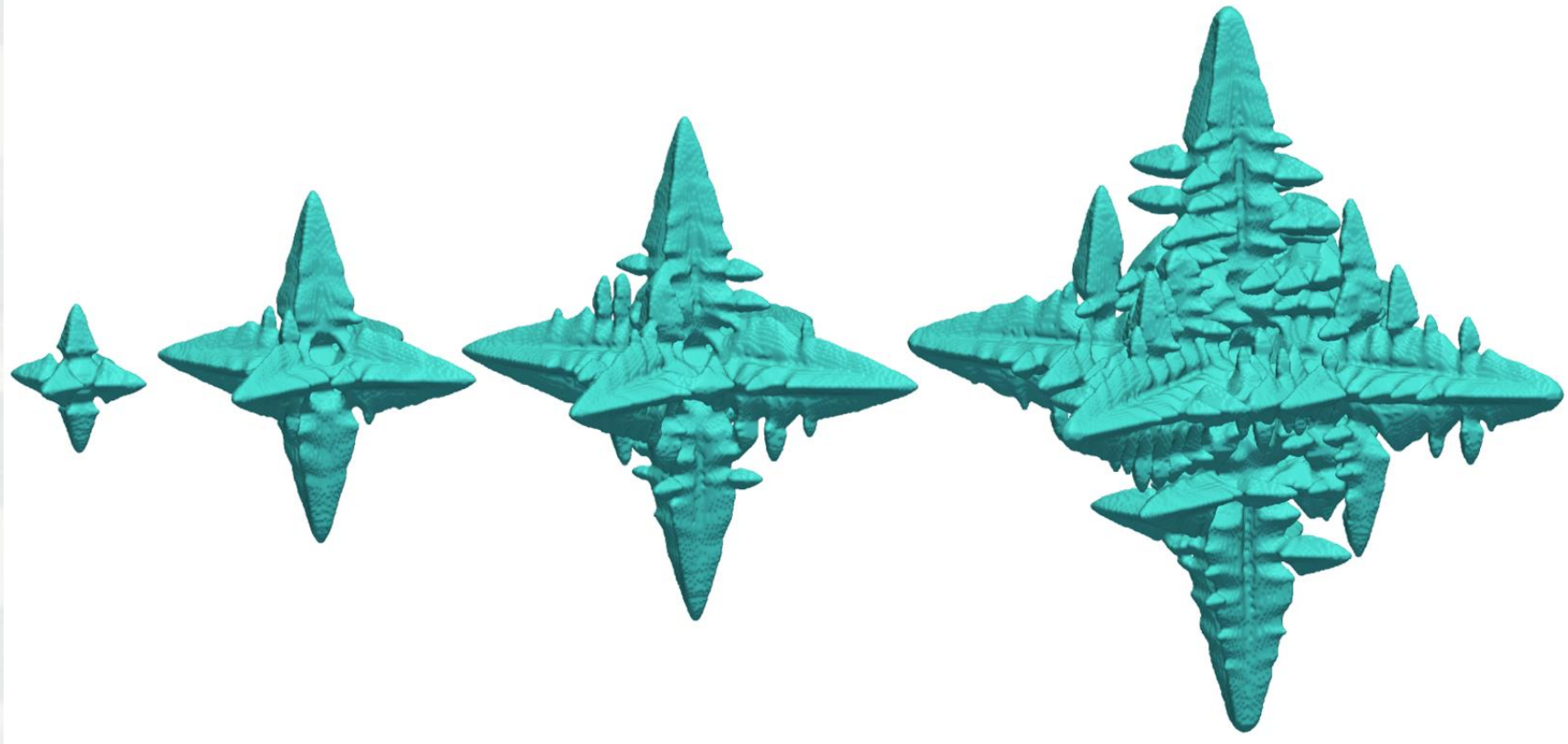
Recently added

- convection (fluid velocity) in parallel
- output stride to reduce data for visualization
- velocity calculation on a coarser subgrid
- measure tip velocity and solute concentration profiles

Planned (as needed)

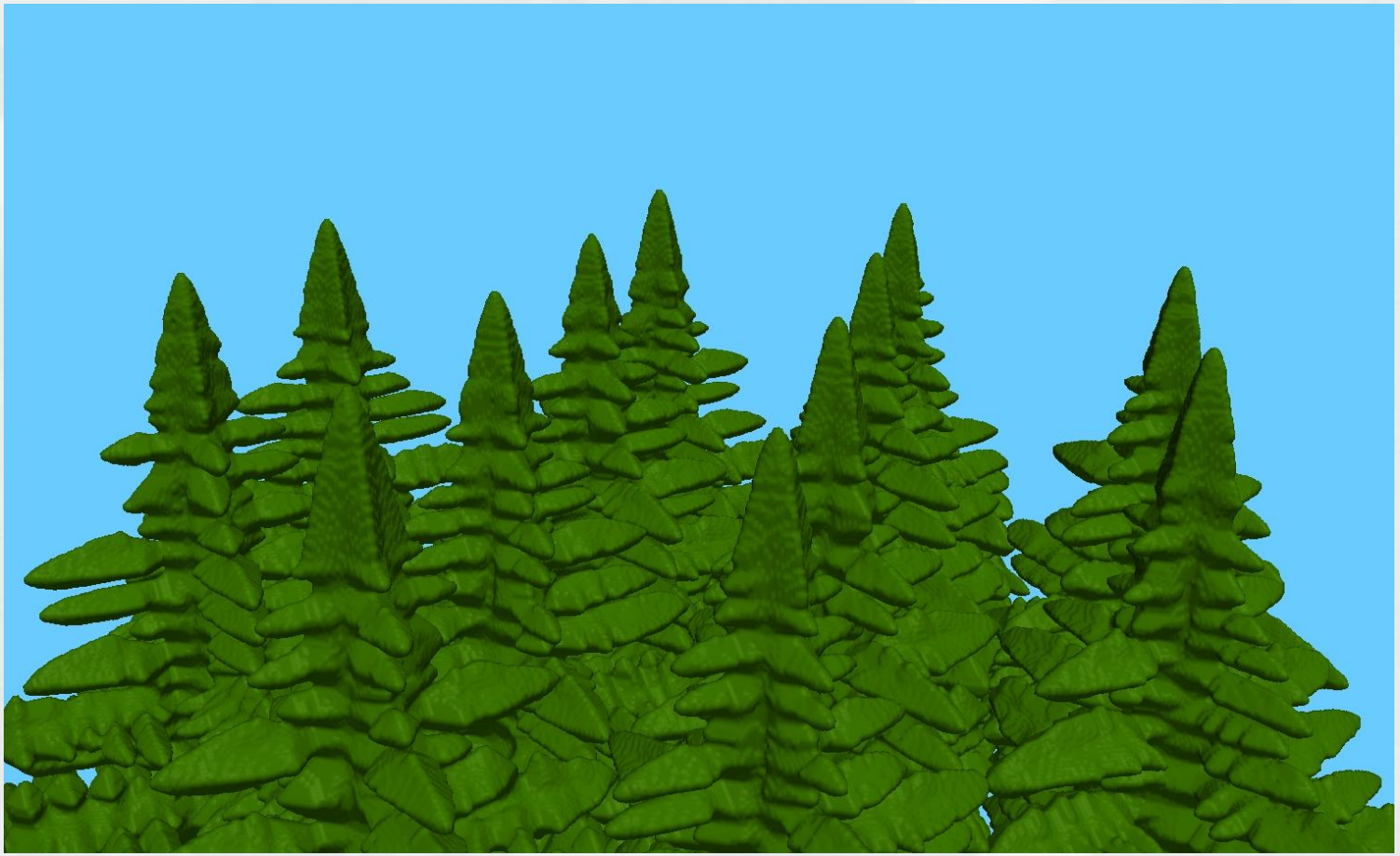
- parallelize full temperature field calculation in 3D

Growth of Al-Cu dendrites in a 120x120x120 μm^3 with 4.5 °C undercooling. From left to right, after 3, 7, 10, and 15 ms [1].



[1] M. Eshraghi, S.D. Felicelli, B. Jelinek, "Three-dimensional simulation of solutal dendrite growth using lattice Boltzmann and cellular automaton methods", Journal of Crystal Growth, Vol 354 (1), pp 129-134, 2012.

Columnar dendrites growing in an undercooled melt of Al-3wt%Cu. Domain size 180x180x144 $(\mu m)^3$



By Mohsen Eshraghi

Publications

Published:

Journal articles:

- Eshraghi, M., Felicelli, S. D., Jelinek, B. (Jun 2012). Three Dimensional Simulation of Solutal Dendrite Growth Using Lattice Boltzmann and Cellular Automaton Methods. Journal of Crystal Growth Elsevier, 354(1), 129-134

In progress:

Journal articles:

- Jelinek, B., Eshraghi, M., Felicelli, S. D., Peters, J. F. Parallel lattice Boltzmann - cellular automaton model of two-dimensional dendritic growth – for Scripta Materialia (4 page limit)
- Jelinek, B., Eshraghi, M., Felicelli, S. D., Peters, J. F. Parallel lattice Boltzmann - cellular automaton model of two-dimensional dendritic growth – for Computer Physics Communications
- Eshraghi, M., Felicelli, S. D., Jelinek, B. A three-dimensional lattice Boltzmann-cellular automaton model for dendritic solidification under convection

Publications

Presentations, accompanied by articles in proceedings:

- Jelinek, B., Eshraghi, M., Felicelli, S. D., (March 2013). Large scale parallel lattice Boltzmann model of dendritic, 2013 TMS Annual Meeting & Exhibition
- Eshraghi, M., Jelinek, B., Felicelli, S. D., (March 2013). A three-dimensional lattice Boltzmann-cellular automaton model for dendritic solidification under convection, 2013 TMS Annual Meeting & Exhibition

Planned:

Journal articles:

- Jelinek, B., Eshraghi, M., Felicelli, S. D., Peters, J. F. Parallel lattice Boltzmann - cellular automaton model of three-dimensional dendritic growth

Conclusions

Accomplishments

- Implemented tests of the strong and weak parallel scaling of LBM/CA model with dendrites at advanced growth stage
- Parallelized velocity in the 3D lattice Boltzmann / cellular automaton model for dendrite growth
- 3D velocity calculation on a coarser subgrid
- Measuring tip velocity and solute concentration profiles

Plans

- Implement LBM-DEM coupling