

High Performance Computing Applications

Presented to: Secretary of Energy
Advisory Board (SEAB)

Fred Streitz, Director
HPC Innovation Center
Lawrence Livermore National Laboratory



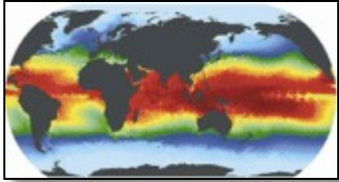
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Lawrence Livermore National Security, LLC



Mission leads us to refine the ability to predict **with confidence** the evolution of complex physical systems



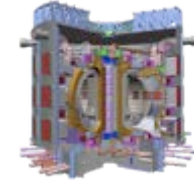
Climate and Weather



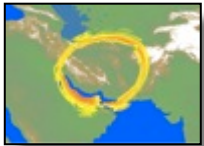
Nuclear deterrence



Combustion



ITER



Nonproliferation

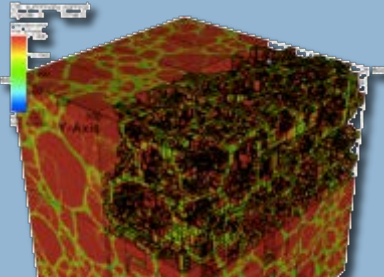


Reactors

Predictive
Integrated
Codes



Medicine



Physics and
Engineering Models



High Performance
Computing

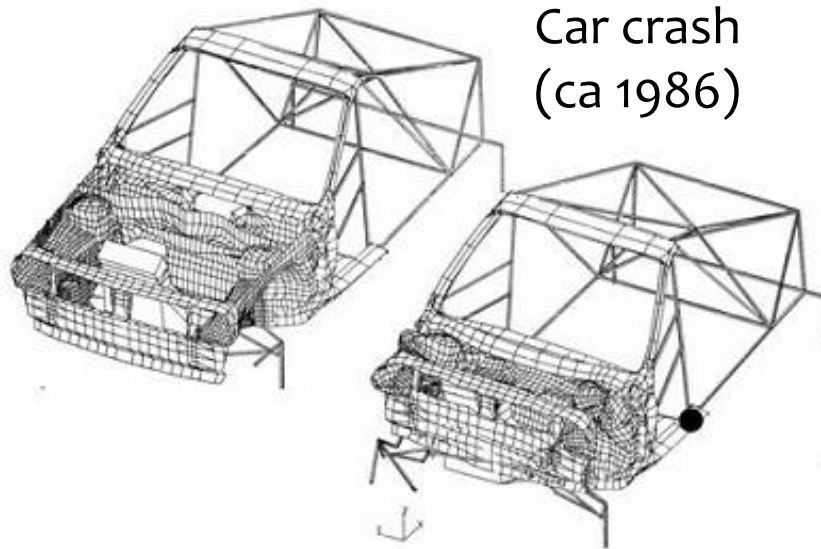


Experimental Validation
and Verification

Simulation is the integrating element of stockpile stewardship

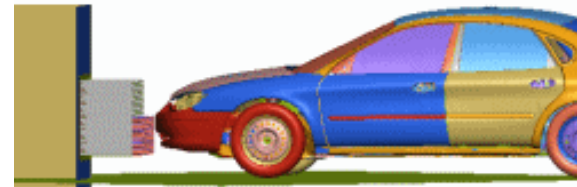
Leading supercomputers are about 5 orders of magnitude more powerful than a desktop computer

Enabling simulations 100,000x more realistic



Car crash
(ca 1986)

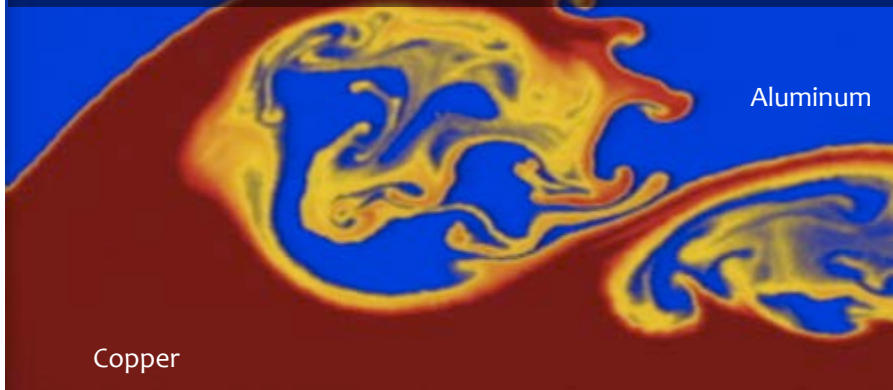
(a) crash simulation



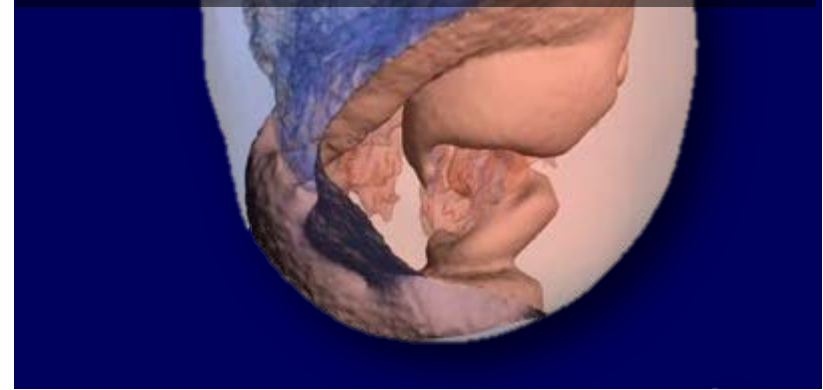
Car crash
(ca 2007)

Ultra-capability computing is disruptive for science and key to creating transformational solutions

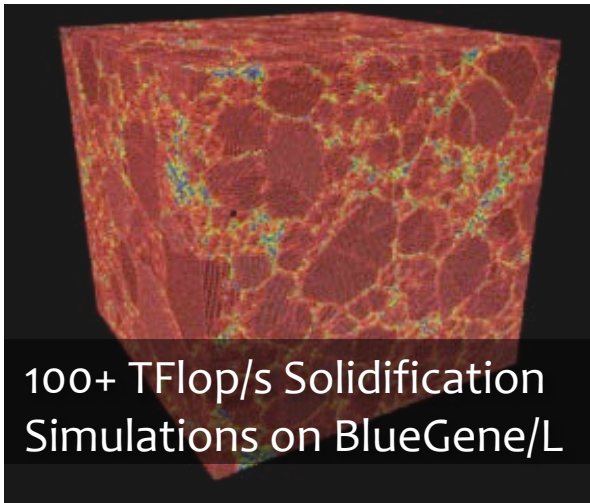
Atom by atom simulation of Kelvin-Helmholtz instability



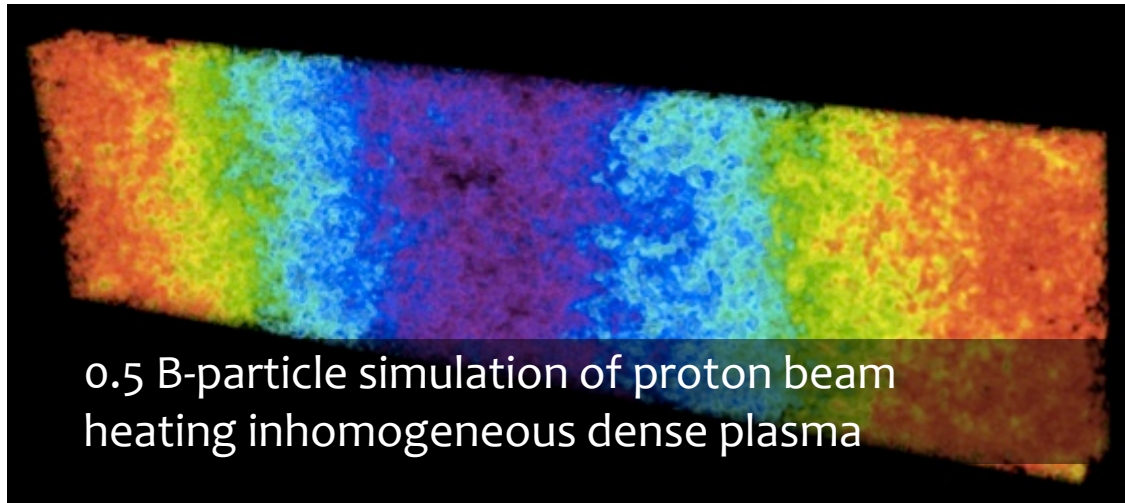
Near real-time simulation of a beating human heart



100+ TFlop/s Solidification Simulations on BlueGene/L

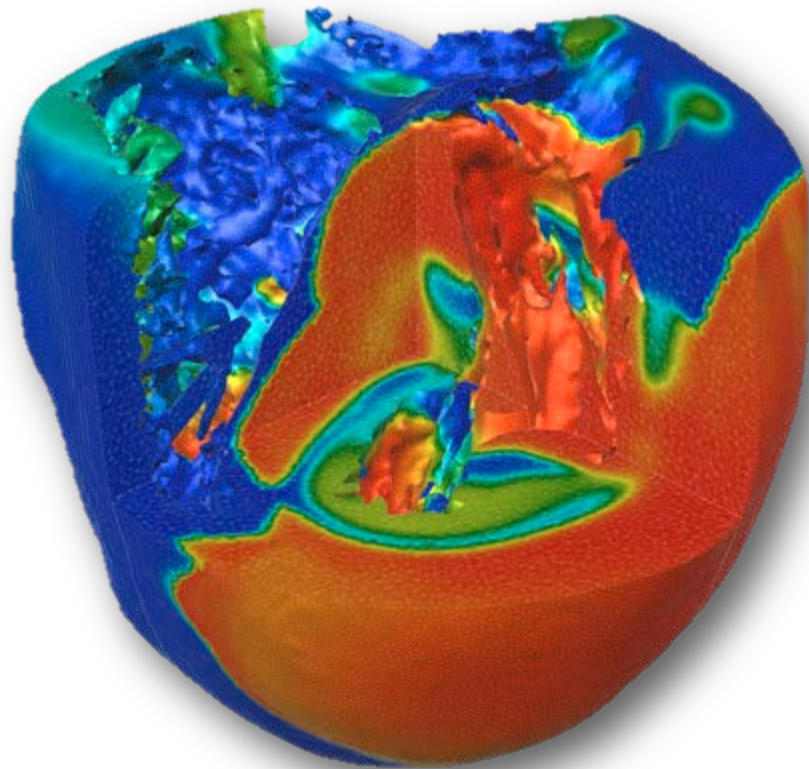


0.5 B-particle simulation of proton beam heating inhomogeneous dense plasma



Whole heart modeling at cellular resolution in real time

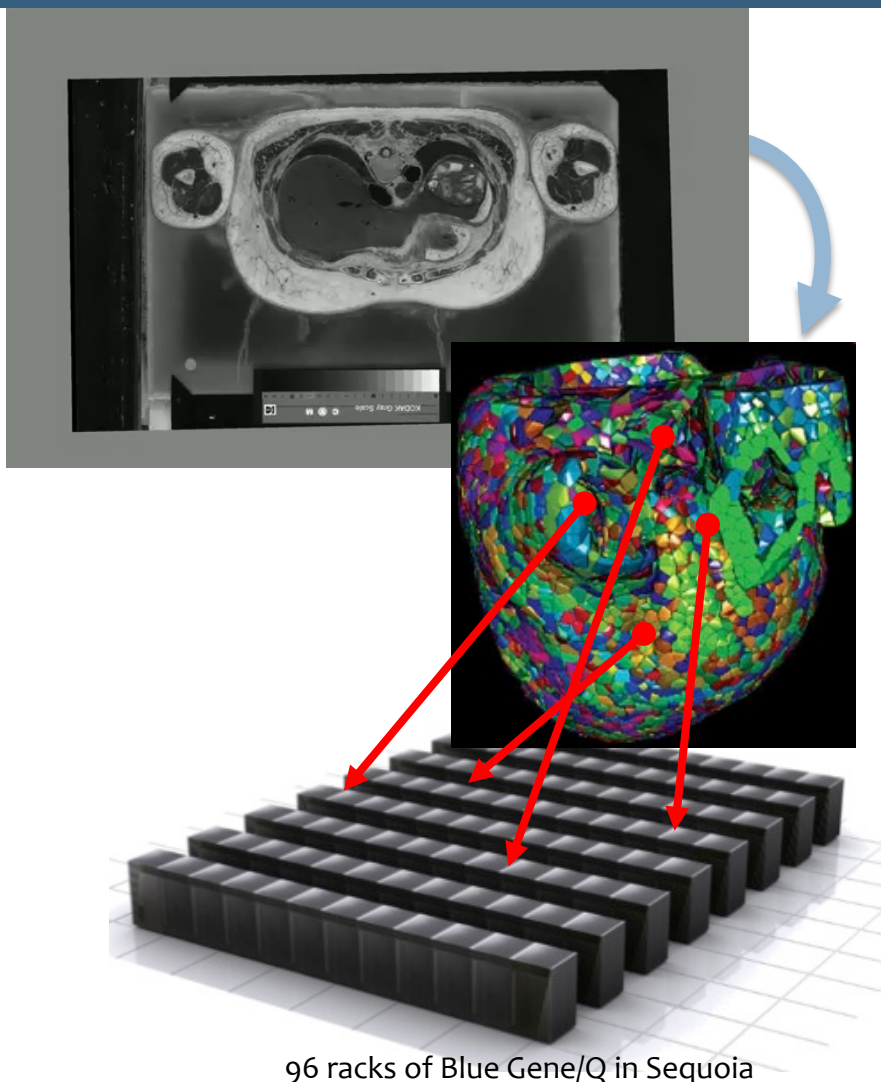
Example of joint capability development



- Bring together multi-disciplinary, multi-institutional team (IBM-LLNL)
- Develop high resolution, realistic model of human heart
- Create *Cardiod* code to model electrophysiology of heart
- Leverage 20 PF Sequoia (Blue Gene/Q) resource
- Investigate development of arrhythmia

- “Bake out” period on new architecture enables discovery-class open science
- Publishable, newsworthy work returns favorable press for DOE and NNSA
- Scaling, load balance and resilience issues are worked out prior to program use

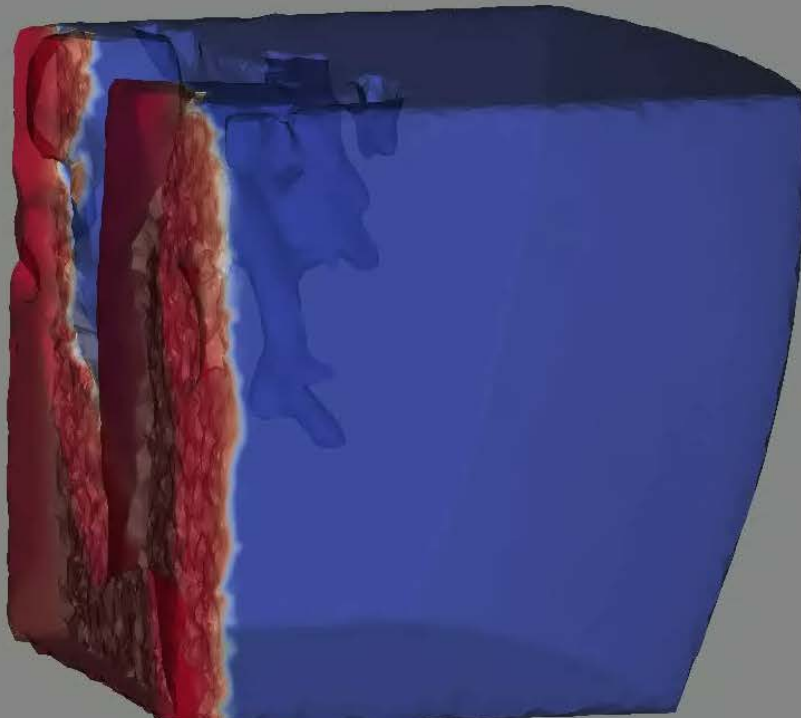
The Cardioid Model on Sequoia



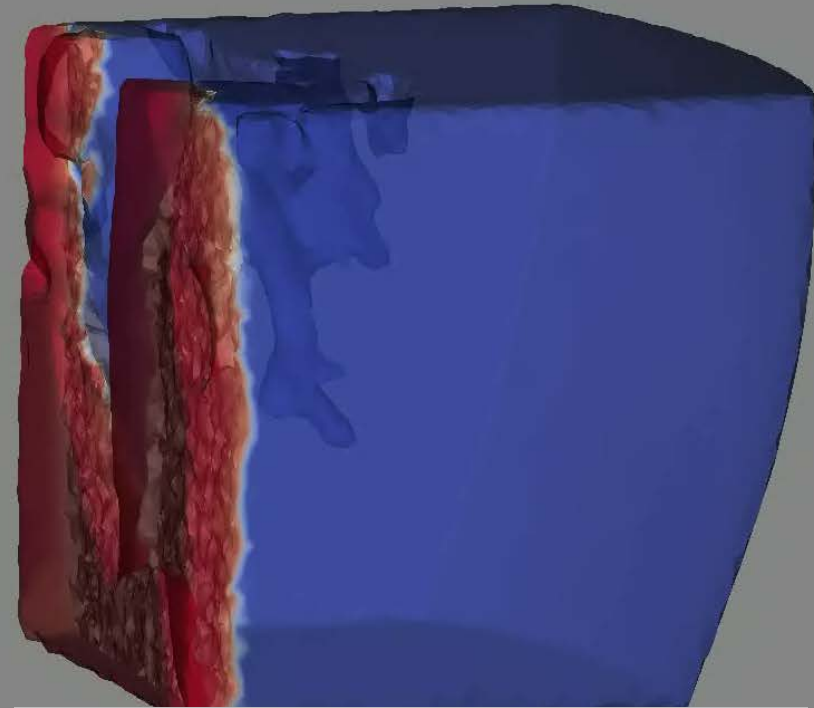
96 racks of Blue Gene/Q in Sequoia

- Complete heart is 370-700 million cells in a complex geometry
- Sub-domains of ~200-500 cells must be mapped to each of 1.6 M cores
- Cell model must be computed on every cell for each time step including reaction and diffusion
- Sub-domains must exchange boundary data on each time step
- Code is written from scratch to take advantage of BG/Q hardware
- Extensive algorithmic improvements
- *1200x faster than nearest competitor*
- 2012 Finalist in Gordon Bell Prize

Heart wedge simulation in presence of d-sotalol



with drug

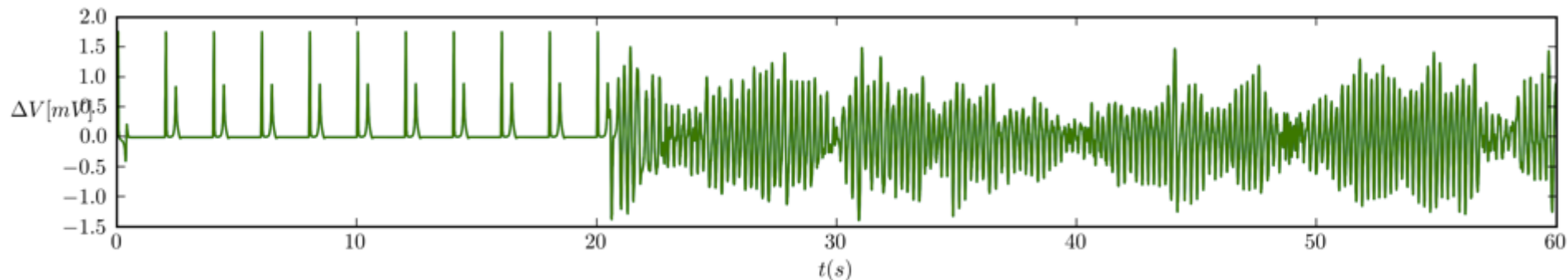


without drug

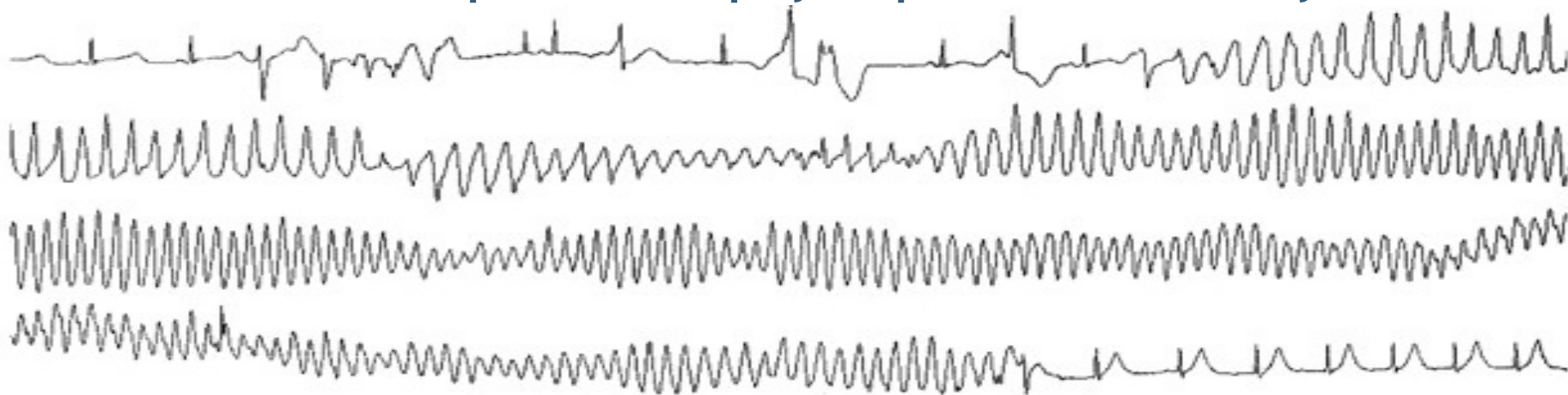
- Drug presence modeled as block to I_{Kr} (hERG) channel
- S1-S2 stimulation protocol introduces transmural reentrant pattern

Supercomputing enables detailed investigation into mechanisms of arrhythmia

ECG calculated from simulation with E-4031



ECG measured in patient with polymorphic ventricular tachycardia



Kobza R et al. Circulation 2005;111:e173-e174

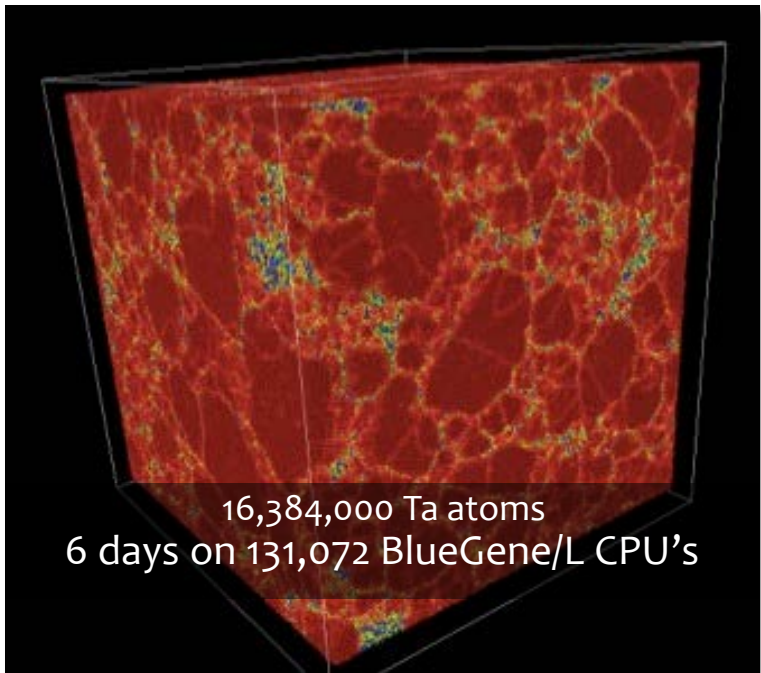
High fidelity model allows previously impossible research directions to unfold

Attracting interest from biomedical industry

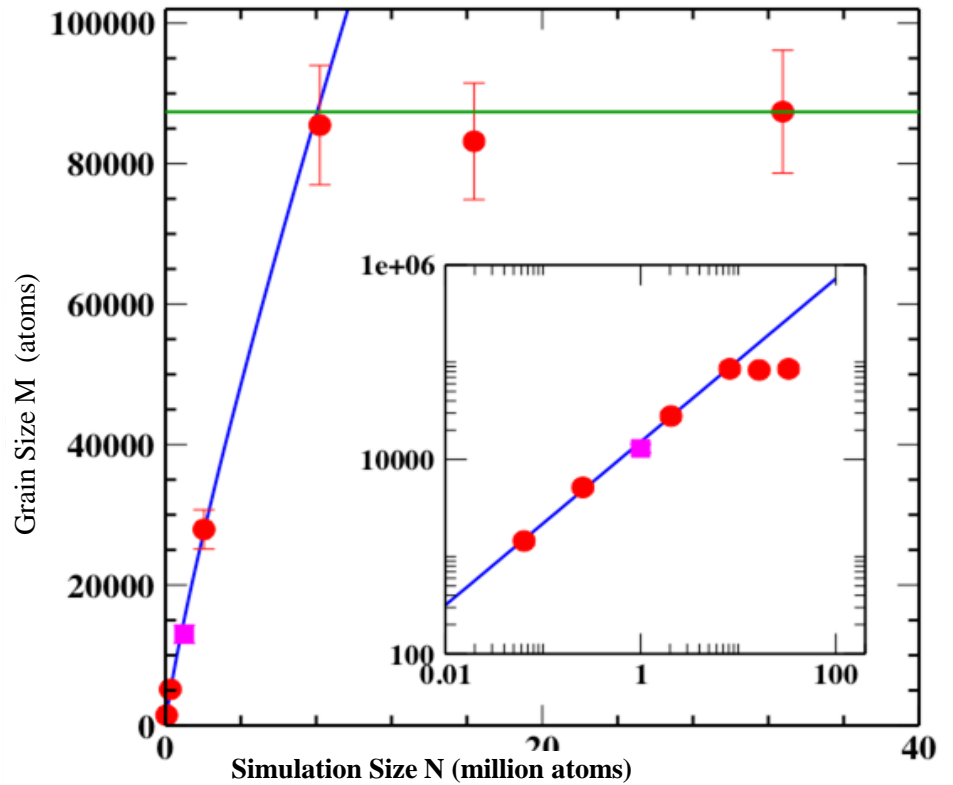
- Drug screening against adverse effects
- Drug discovery/design
- Optimum drug dosage
- Cardiac ablation for arrhythmia
- Cardiac device placement and settings



Capturing the metal solidification process

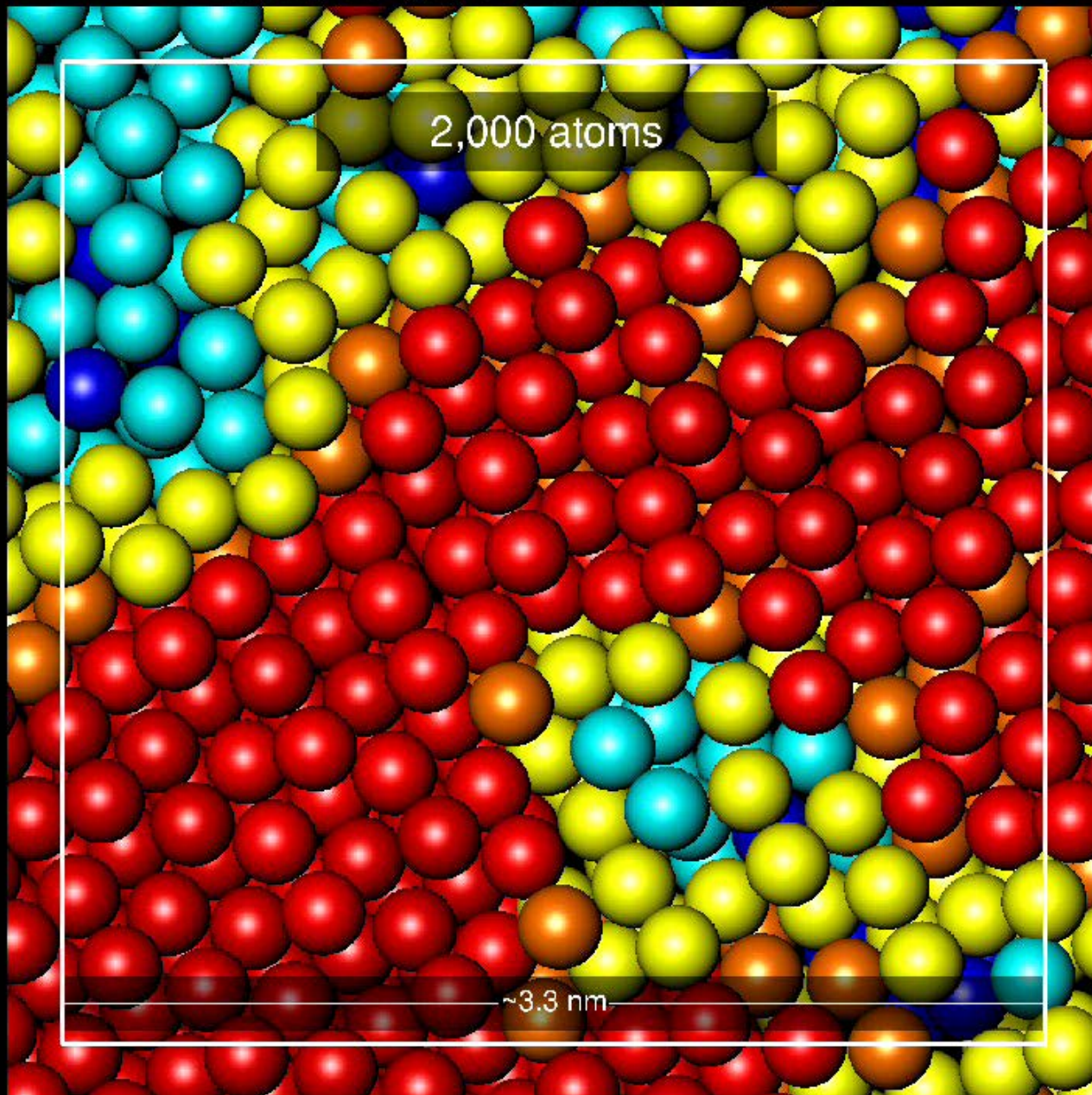


- Need 10's of millions of atoms to accurately model the formation of grains solidifying from a melt
- Solidification is a process crucial to some additive manufacturing processes

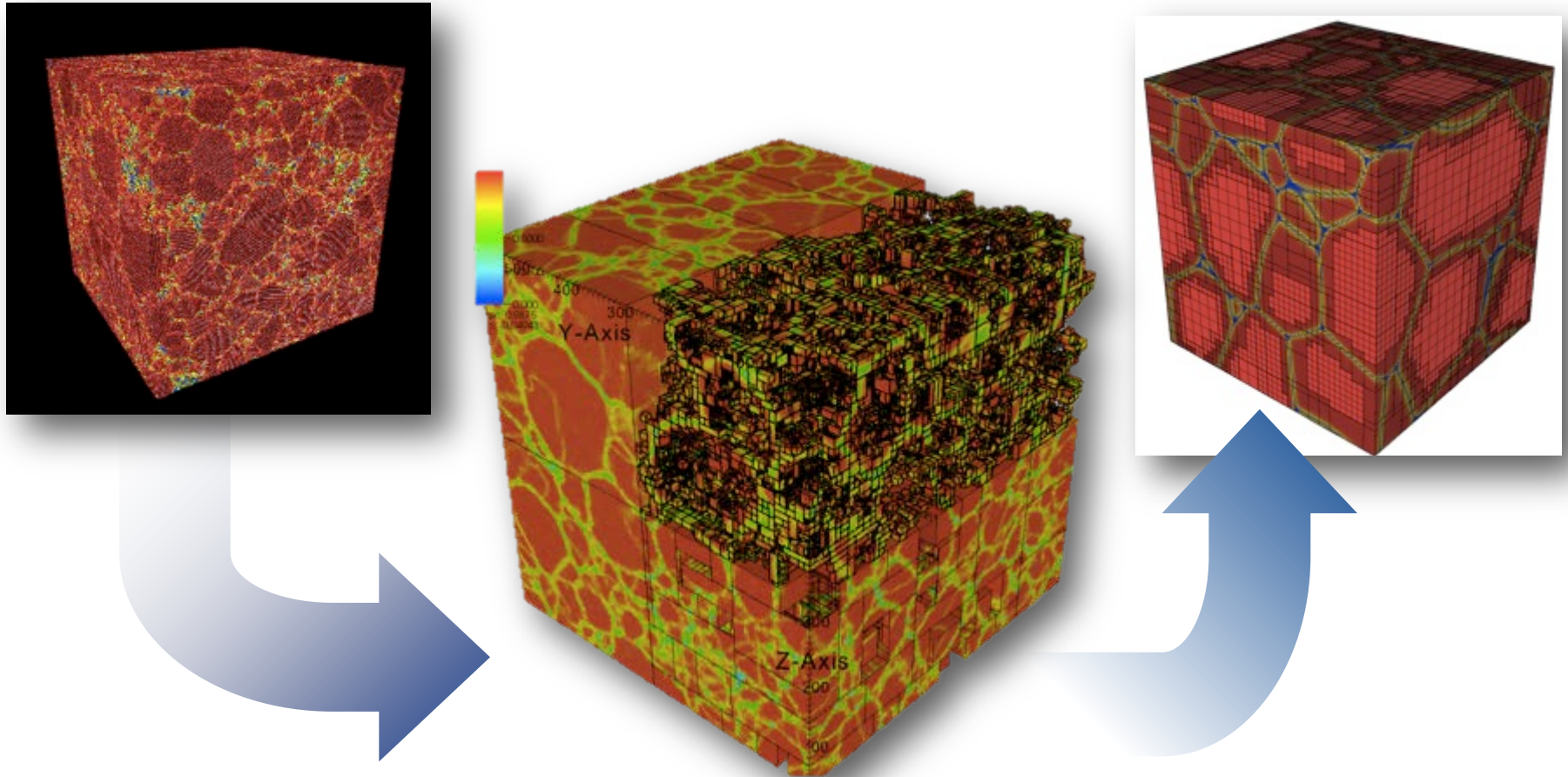


Smaller simulations produce incorrect (and uncorrectable) results!

Pressure-induced Solidification in MGPT Tantalum
modeled using ddcMD code on BlueGene/L



Realistic simulation of solidification is the starting point for investigation of coarsening



Resulting microstructures extracted from MD simulations can be used as initial conditions for phase field modeling of subsequent evolution

Exascale computing is required to access realistic scales of either of length or time with realistic materials models

