CoHMM

Co-design proxy app for the Hierarchical Multiscale Method

http://github.com/exmatex/CoHMM

Based on a well studied model that represents the basic workload of multiscale simulation.

Vehicle for exploring new *adaptive sampling* algorithms

B. Rouet-Leduc et. al, *Spatial Adaptive Sampling in Multiscale Simulation,* Comp. Phys. Comm. **185**, 1857–1864 (2014)

D. Roehm et. al, *Distributed Database Kriging for Adaptive Sampling*, in preparation

Kipton Barros, kbarros@lanl.gov

LA-UR-14-2774

HMM — Elastodynamics application

Macroscale conservation laws *(Elastodynamics)*

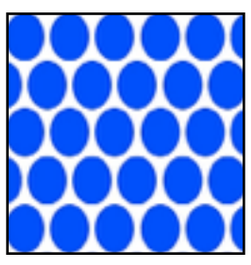
deformation gradient $\partial_t \mathbf{A} = \nabla \cdot \mathbf{v}$

momentum $\rho \partial_t \mathbf{v} = \nabla \cdot \sigma(e, \mathbf{A})$

energy $\partial_t e = \nabla \cdot \mathbf{j}(e, \mathbf{A})$

$$\boxed{\begin{aligned} \mathbf{A} &= \nabla \mathbf{u} \\ \mathbf{v} &= \partial_t \mathbf{u} \end{aligned}}$$

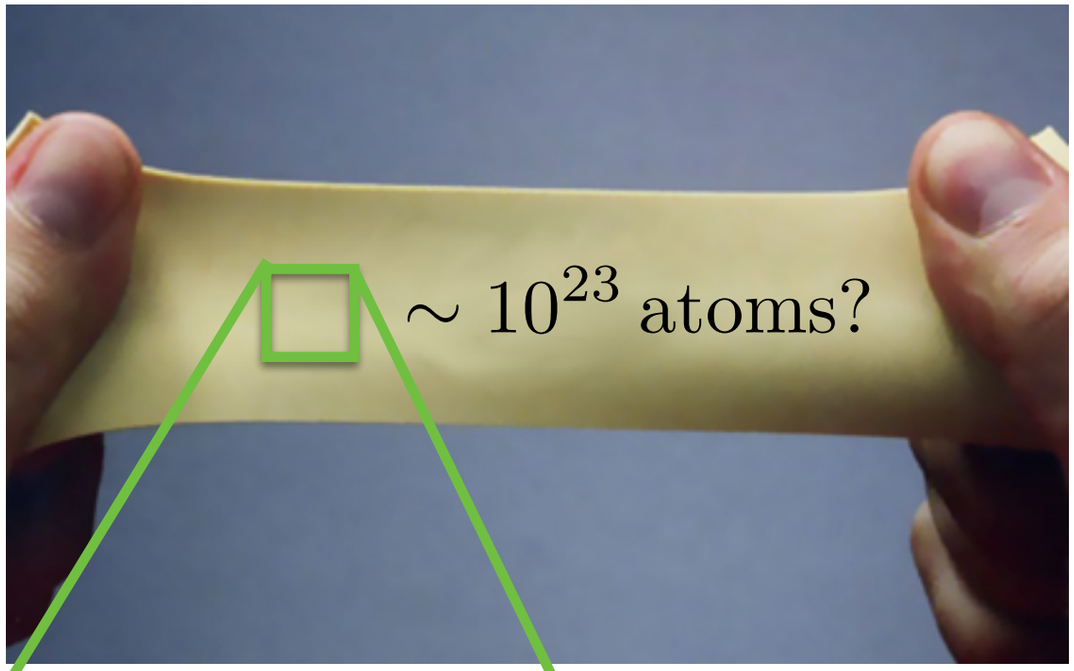
$\sigma(\mathbf{A}, e)$ $\mathbf{A}, e$

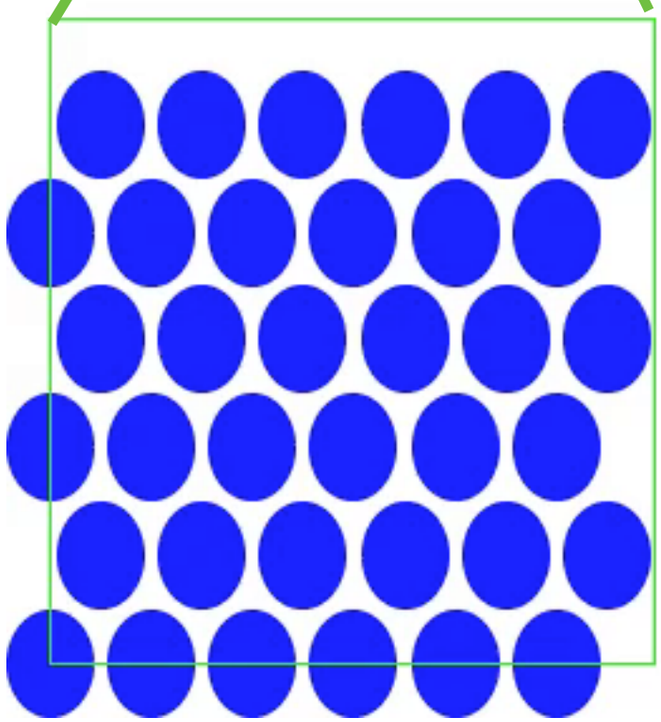


Microscale physics
(Molecular dynamics)

$$m \partial_t^2 \mathbf{x}_i = \mathbf{F} = -\nabla_{\mathbf{x}_i} V$$

deformation gradient $\mathbf{A}$ = *"stretch"*

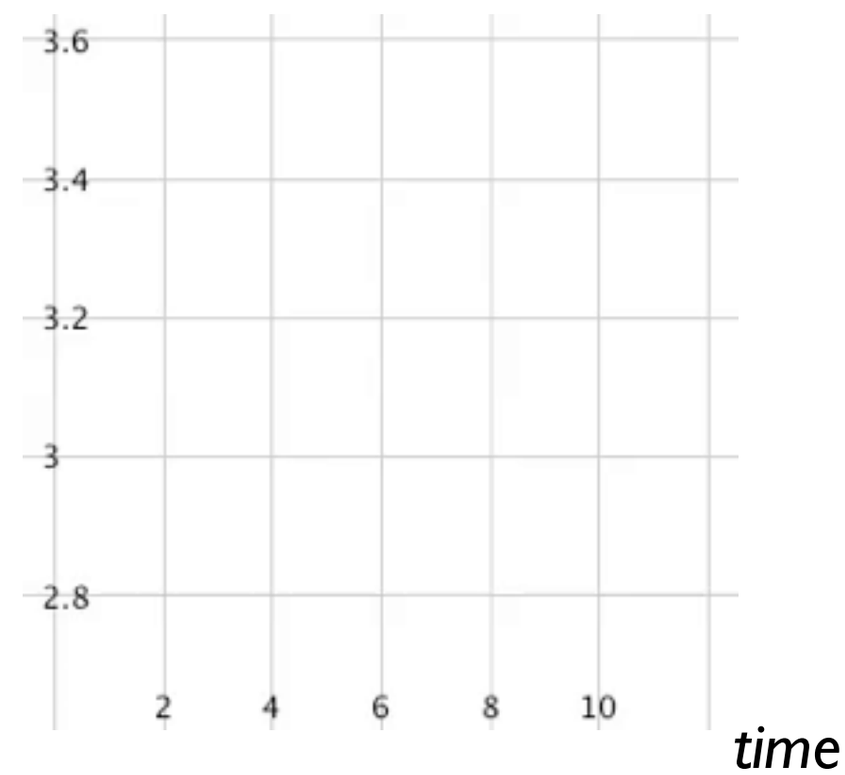




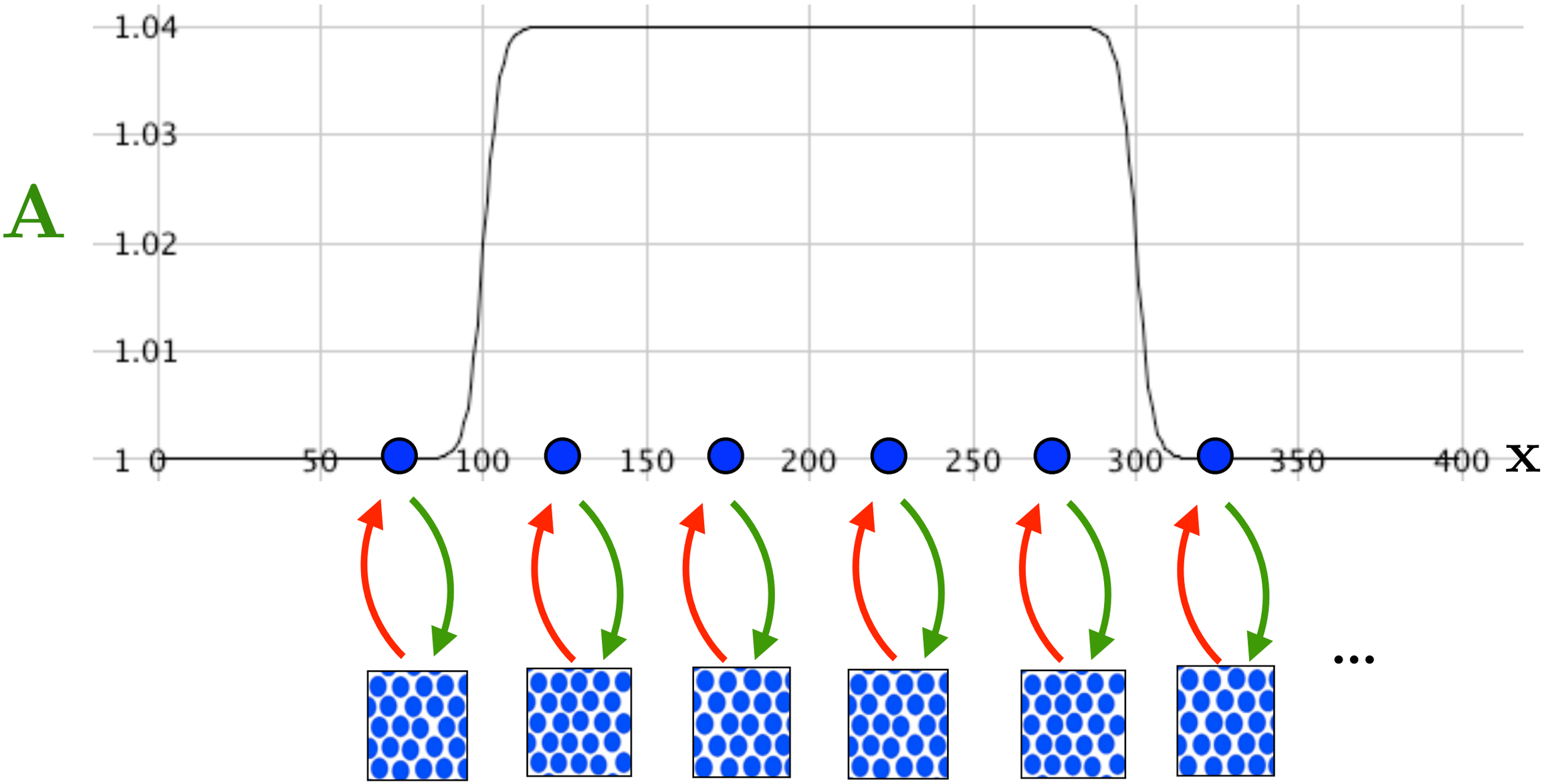
(CoMD with $\sim 10^3$ atoms*)*

$\sigma(\mathbf{A}, e)$

avg. stress



Multiscale simulation



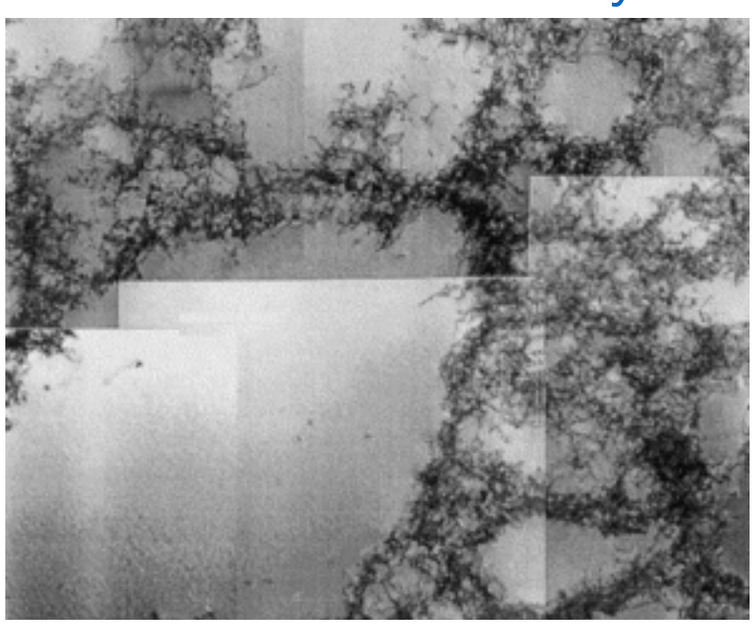
KEY ASSUMPTIONS in scale bridging models:

ergodicity & separation of (time, space) scales

Stress is unique function of macro-state, e.g. $\sigma(\mathbf{A}, e)$

Real materials have defects that couple **many** scales —
a research topic that might tie into our UQ efforts?

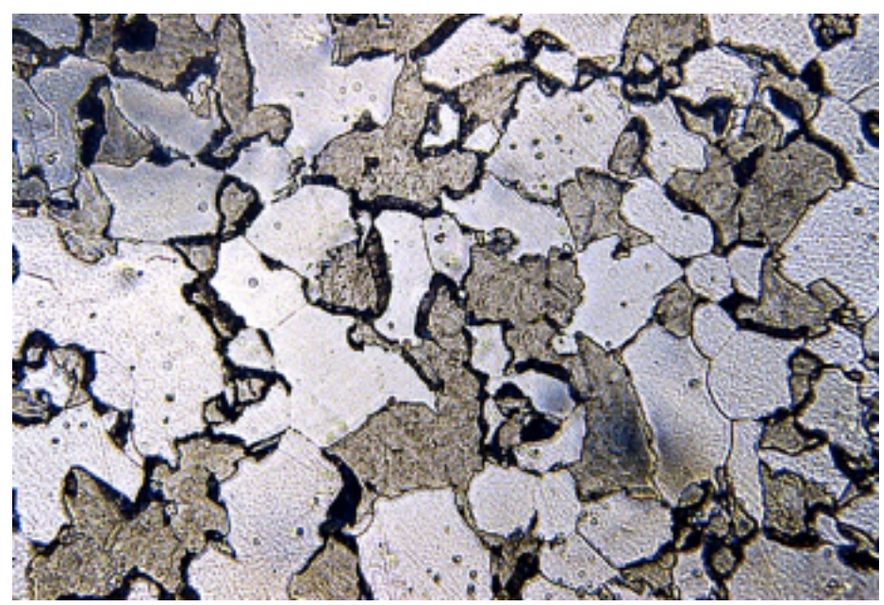
dislocation density



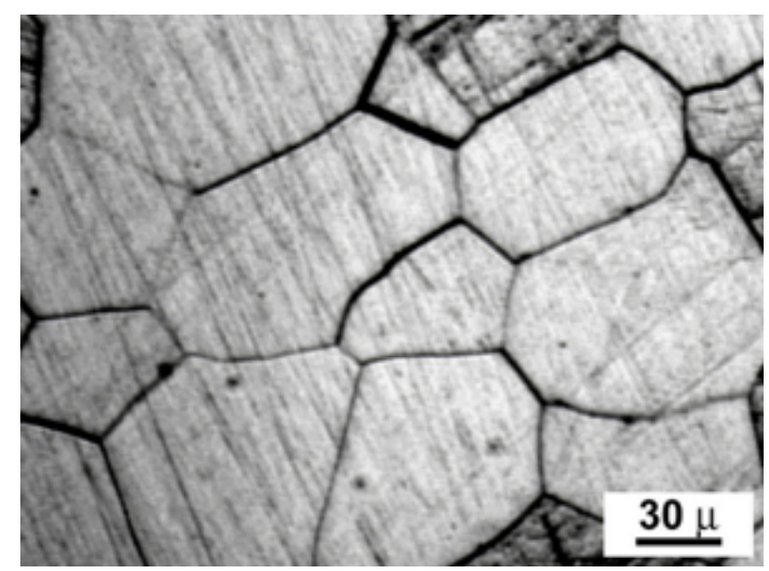
The flow stress of fractal dislocation arrangements

Michael Zaiser[a], Peter Hähner[b]

martensitic microstructure

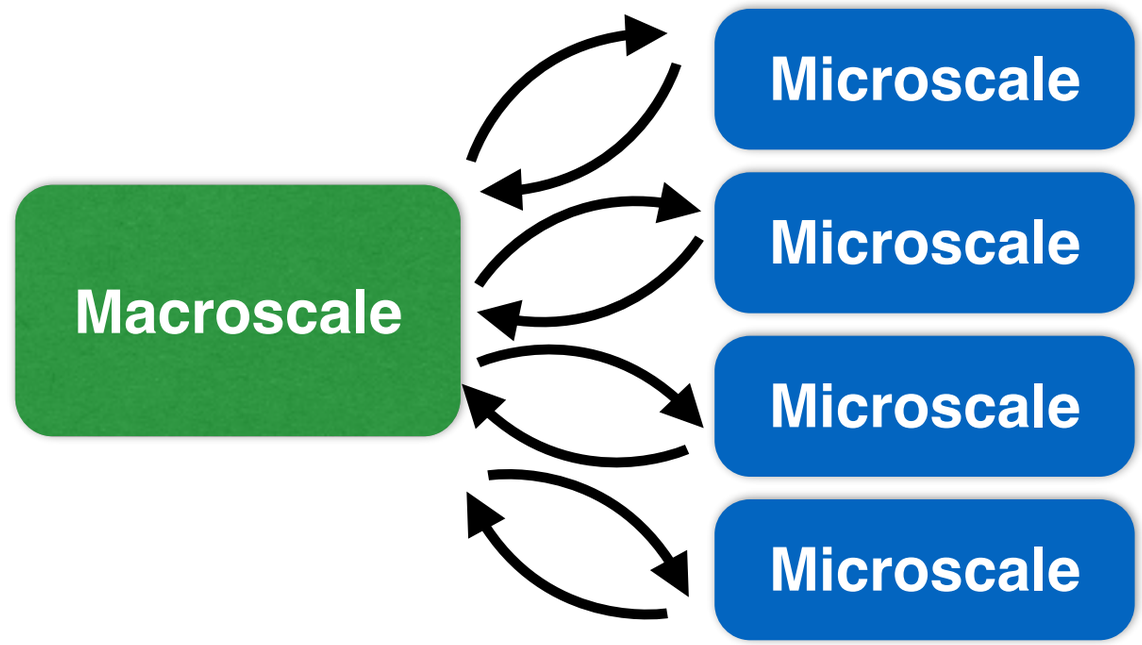


grain boundaries



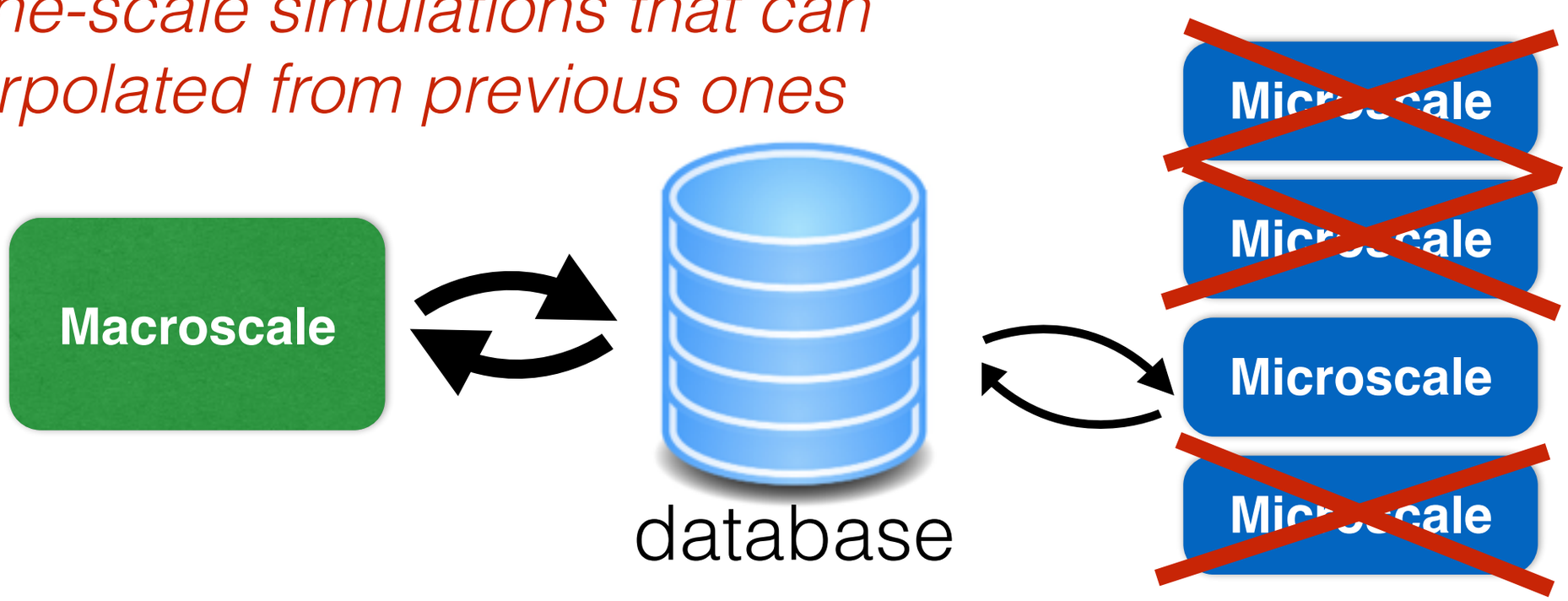
CoHMM workload resembles more complicated models, enables adaptive sampling algorithm design.

Naive multiscale



Adaptive Sampling:

Avoid fine-scale simulations that can be interpolated from previous ones



N. R. Barton et al. *A call to arms for task parallelism in multi-scale materials modeling.* Int. J. Num. Methods. Eng., **86**, 744–764 (2011)

Distributing a database at Exascale will be difficult.

LLNL observation:

Most database "hits" are local in space and time

(N. Barton and collaborators)

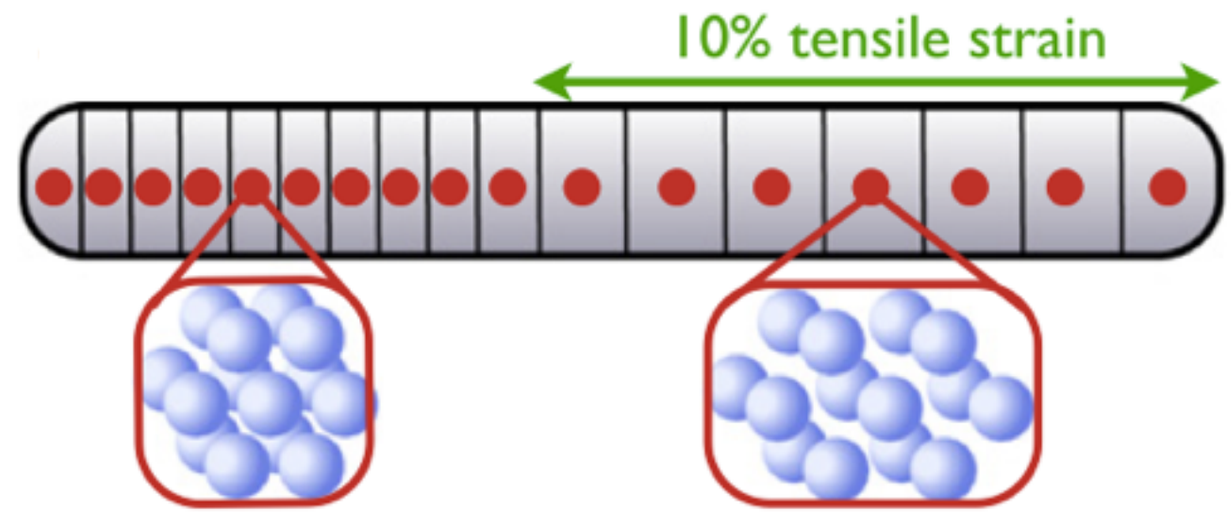
Small step: Cache samples locally to reduce synchronization with global database.

Extreme step: **Eliminate global database**, interpolate using local information only.

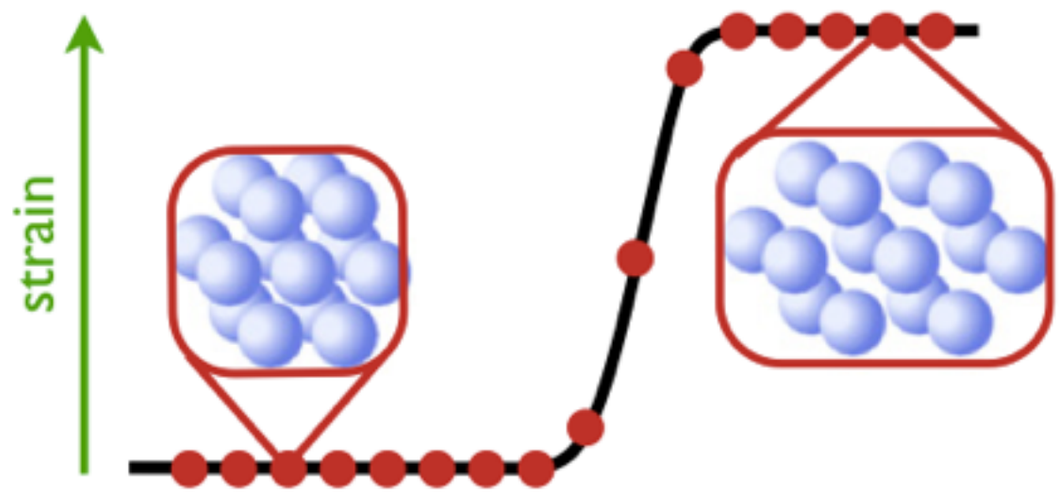
→ ***Spatial*** *Adaptive Sampling*

B. Rouet-Leduc et. al, *Spatial Adaptive Sampling in Multiscale Simulation,* Comp. Phys. Comm. **185**, 1857–1864 (2014)

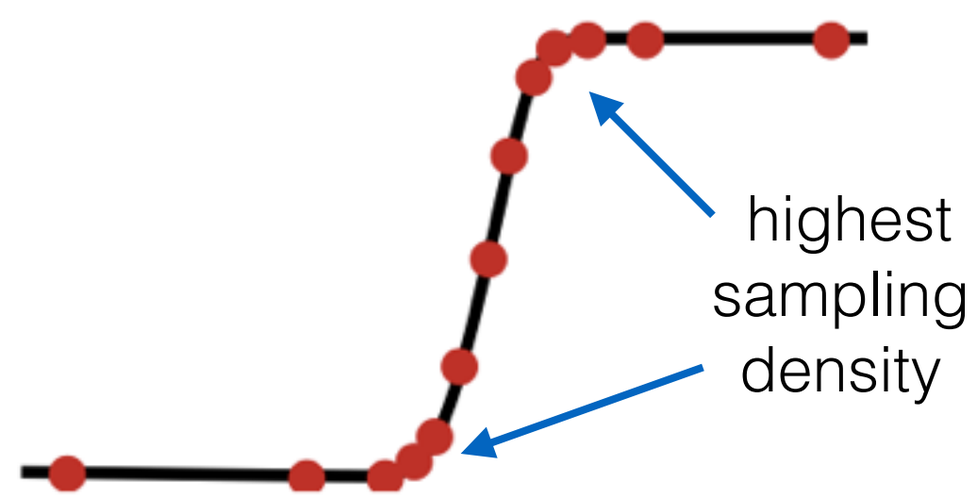
Multiscale simulation



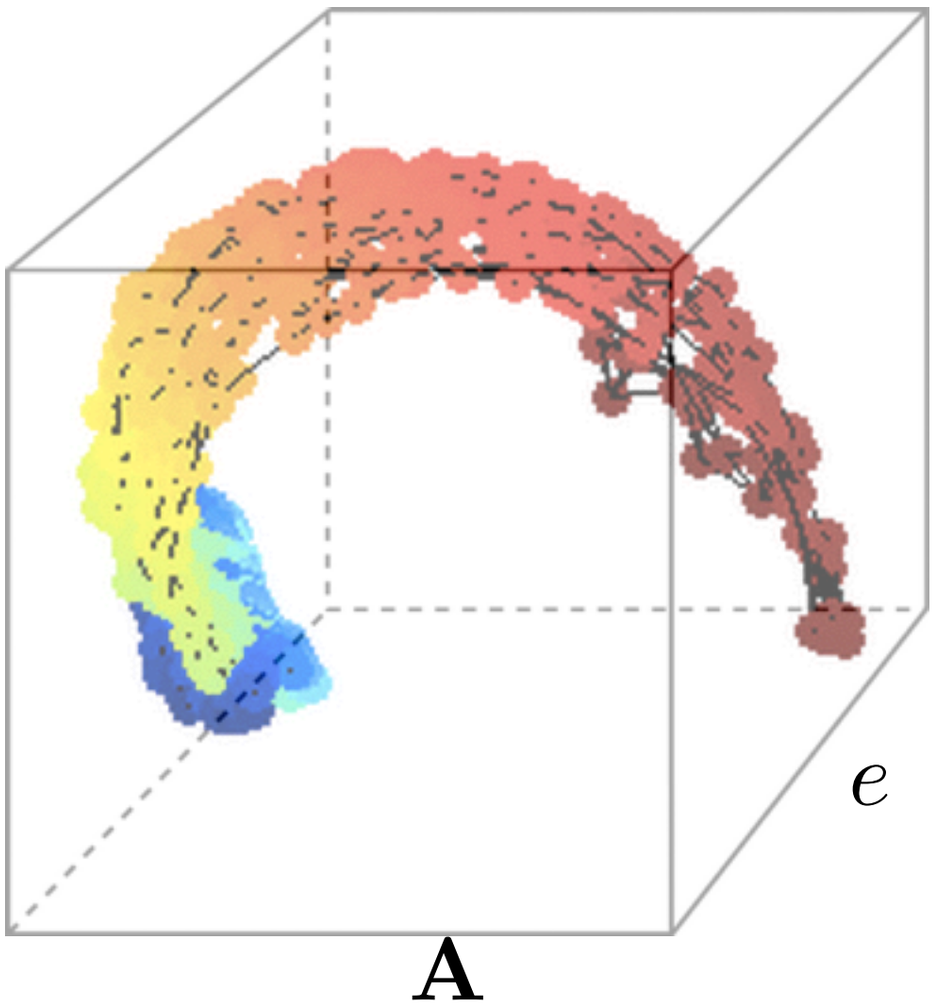
Typically, one evaluates microscale response on uniform macro-grid



Spatial adaptive sampling
reconstructs stress field by spatially interpolating carefully selected sample points

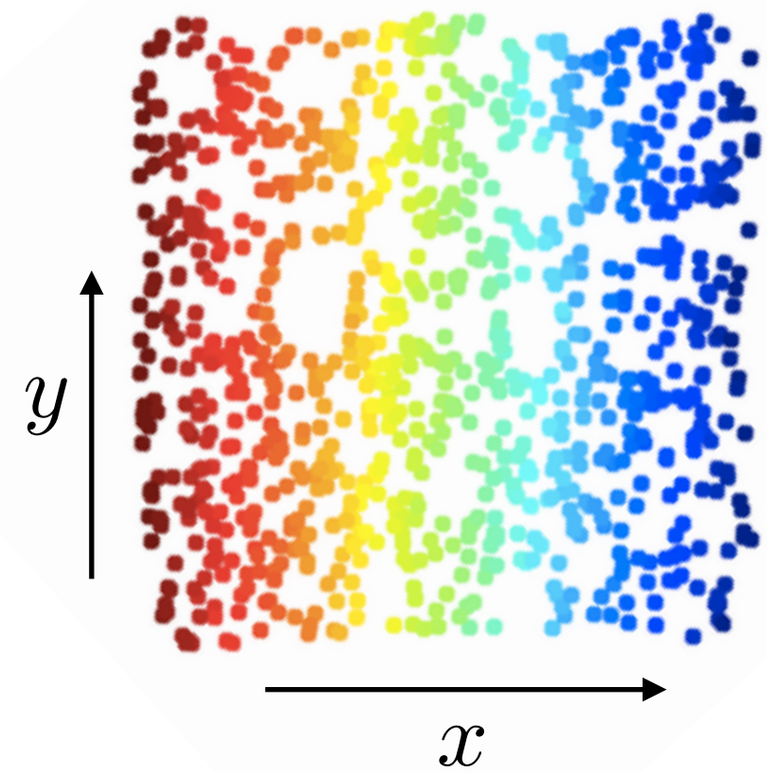


Standard adaptive sampling



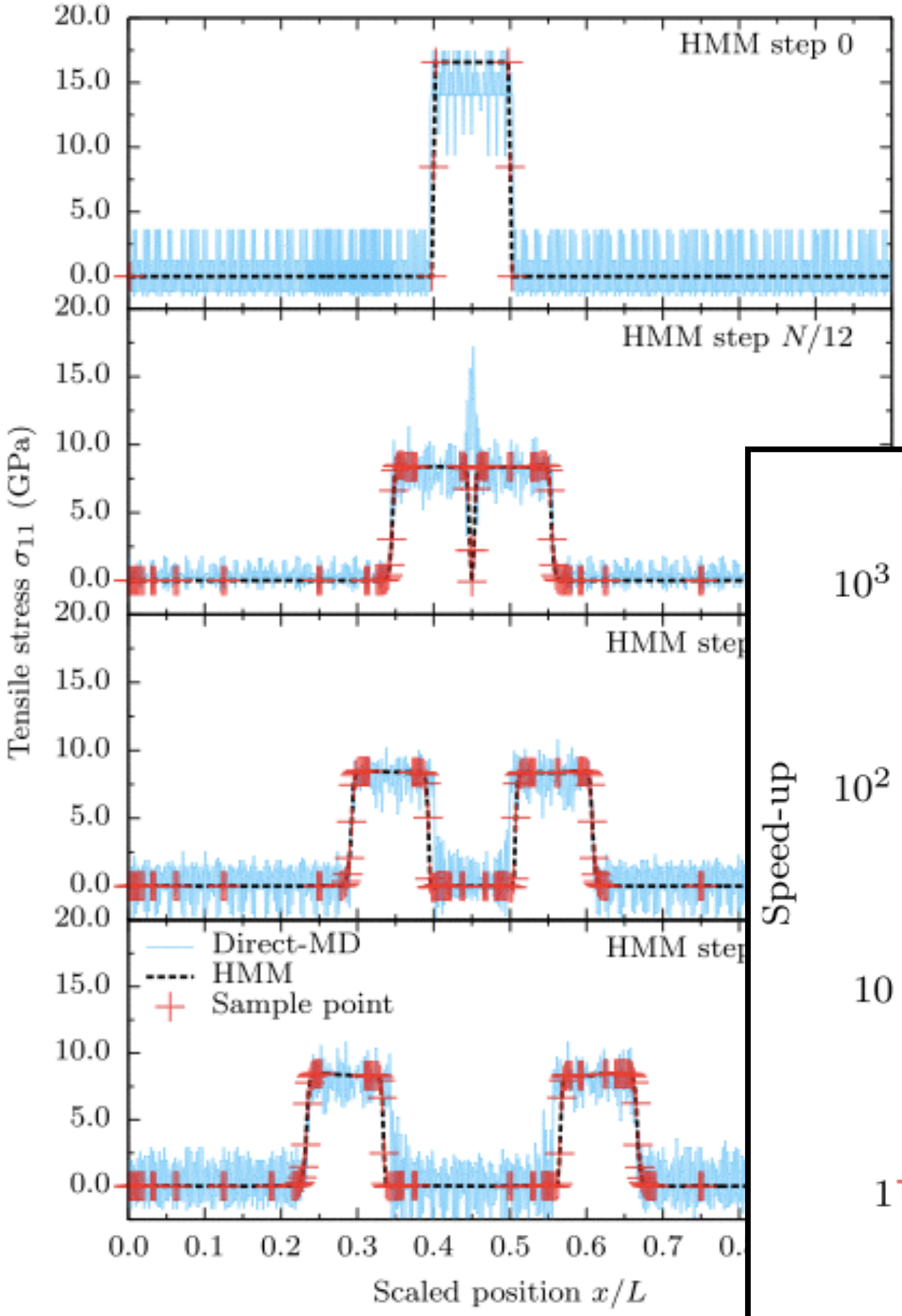
Interpolate in potentially very high-dimensional configuration space

Spatial adaptive sampling



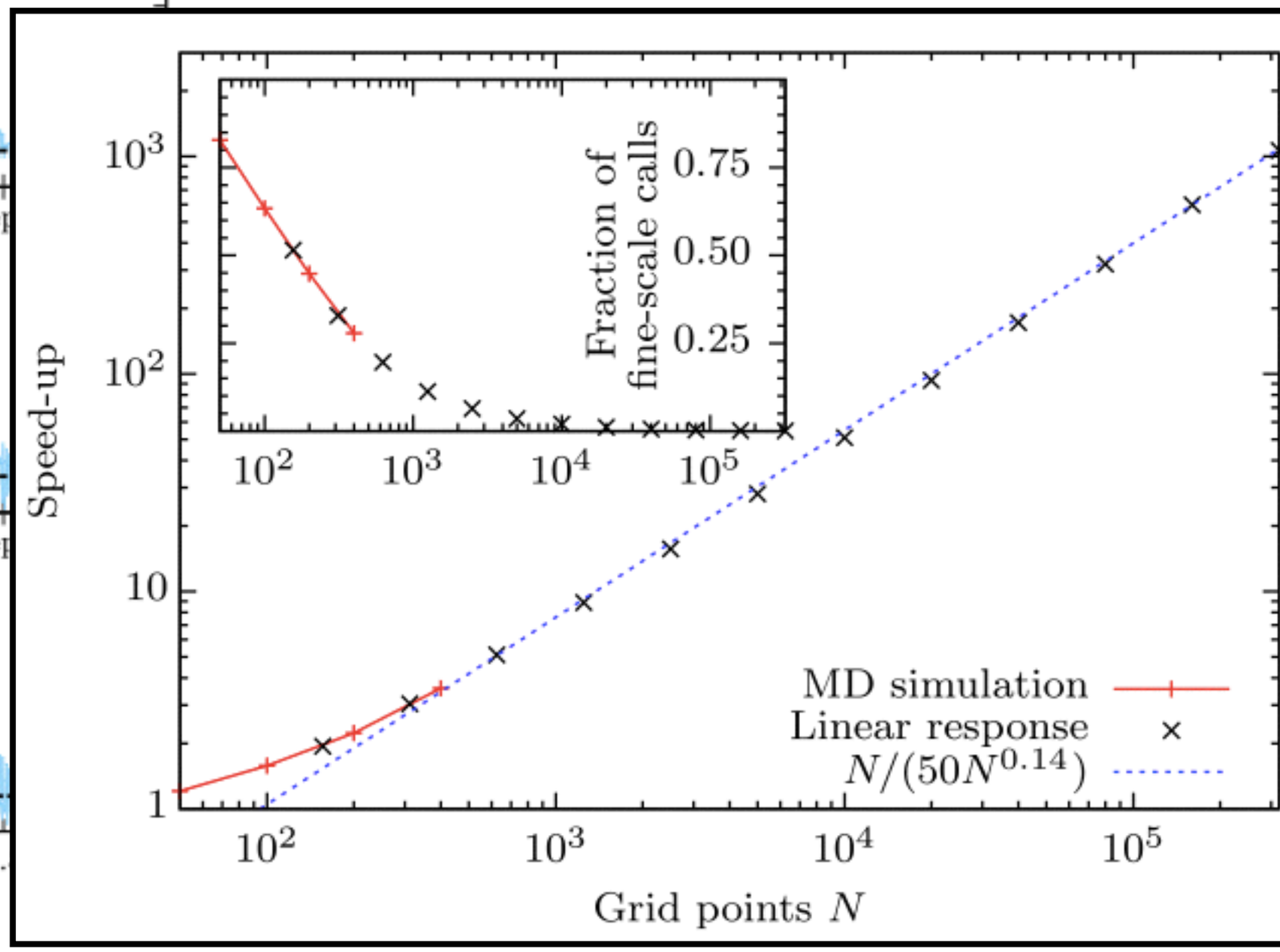
Interpolate in physical d=3 space

Almost all computation focused on shock front.



For certain problems, huge speed-ups possible

B. Rouet-Leduc et. al, *Spatial Adaptive Sampling in Multiscale Simulation,* Comp. Phys. Comm. **185**, 1857–1864 (2014)

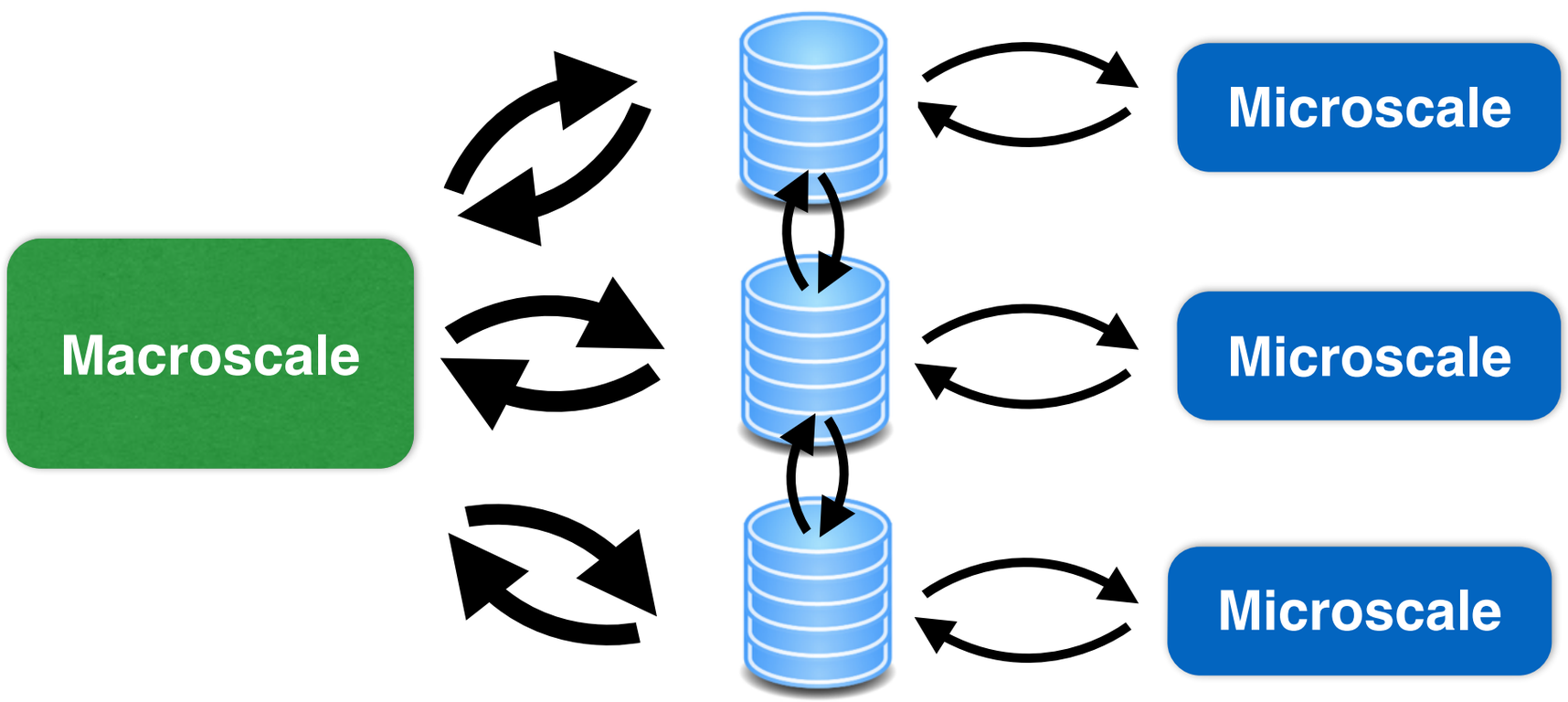


Investigations into ***Distributed*** Adaptive Sampling

D. Roehm et. al, *Distributed Database Kriging for Adaptive Sampling*, in preparation

inspired by

N. R. Barton et al. *A call to arms for task parallelism in multi-scale materials modeling.* Int. J. Num. Methods. Eng., **86**, 744–764 (2011)



distributed database

Technologies

"Ordinary" Kriging interpolation with spherical variograms

robust to stochastic error, and offers confidence intervals

N. Cressie, The origins of kriging, Mathematical Geology 22 (3) (1990) 239–252.

Encoding of keys to index cells in high dimensional sample space

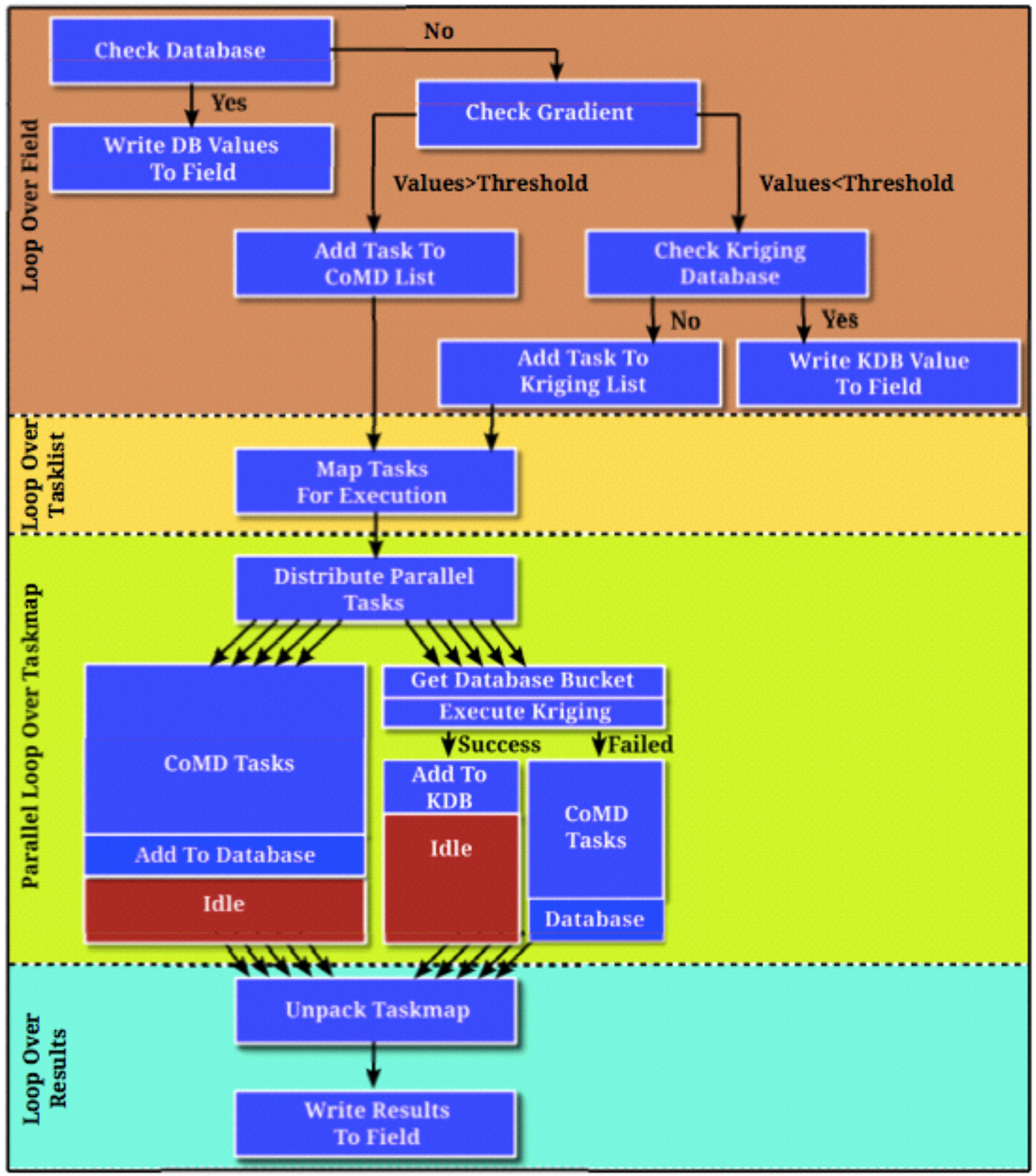
Charm++ runtime

Redis distributed NoSQL database

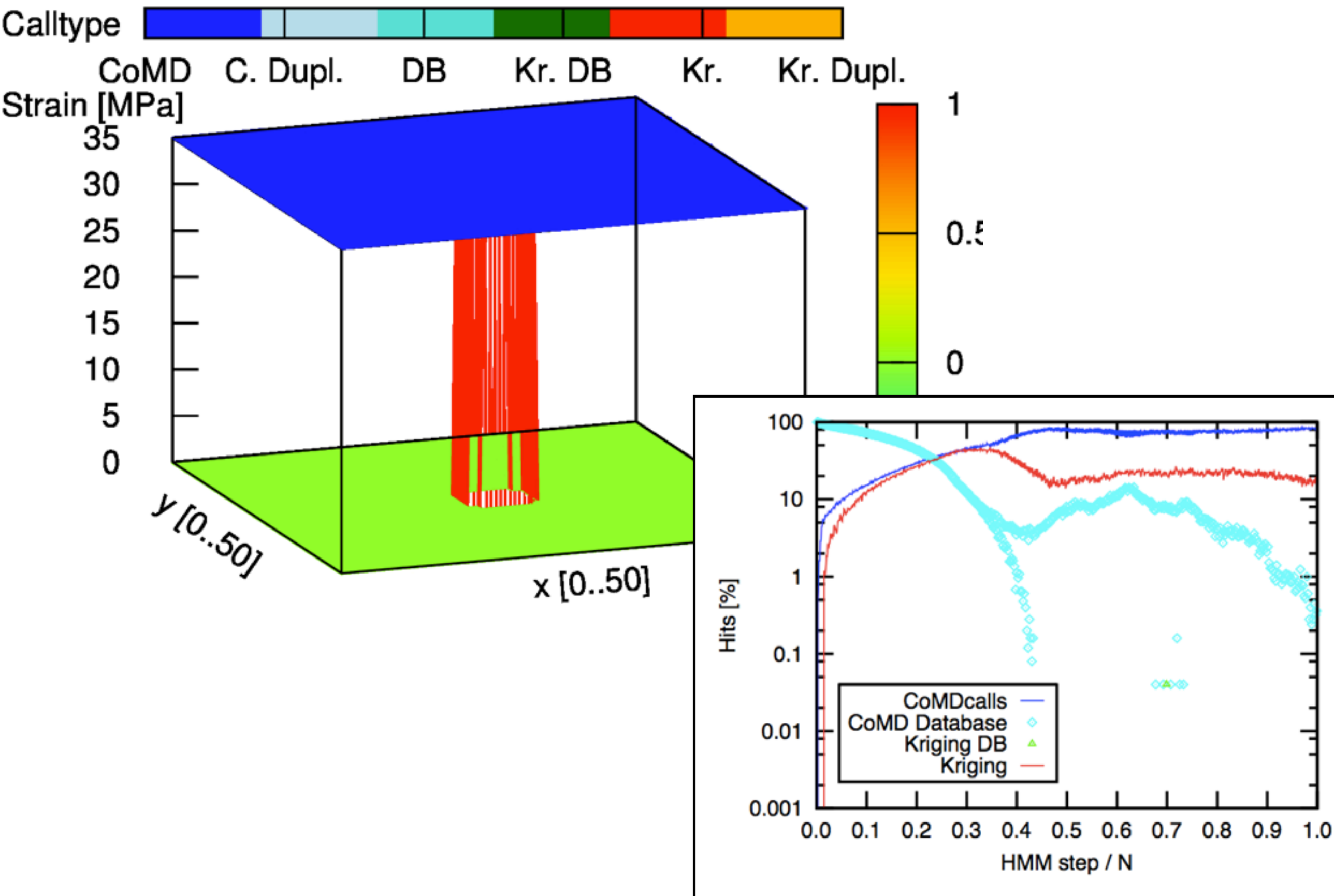
open source
widely used (GitHub, Twitter, Stackoverflow, …)
fault tolerant distribution with "cluster" mode

D. Roehm et. al, *Distributed Database Kriging for Adaptive Sampling*, in preparation

Flow chart


Loop Over Field
Check Database
No
Yes
Write DB Values To Field
Check Gradient
Values>Threshold
Values<Threshold
Add Task To CoMD List
Check Kriging Database
No
Yes
Add Task To Kriging List
Write KDB Value To Field
Loop Over Tasklist
Map Tasks For Execution
Parallel Loop Over Taskmap
Distribute Parallel Tasks
CoMD Tasks
Add To Database
Idle
Get Database Bucket
Execute Kriging
Success
Failed
Add To KDB
Idle
CoMD Tasks
Database
Loop Over Results
Unpack Taskmap
Write Results To Field

Up to 5-25x speedup



Next steps:

Vehicle for testing runtime systems & databases

Christoph Junghans tomorrow @ 9am

Locality sensitive hashing

"One of the biggest CS breakthroughs in recent decades" - P. Hanrahan

Fast nearest-neighbor samples points in high-dimensional space, taming the "curse of dimensionality"

Parallel approaches, e.g. http://istc-bigdata.org/plsh

UQ treatment of scale-separation violations?

Existing methods resolve non-ergodic defects in full atomistic detail

Can we do better by inferring coarse-grained dynamical models using a machine-learning type approach?