Large-Scale DSMC Simulations ...
Part 2: Computational aspects

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Center for Computing Research

Engineering Sciences Center

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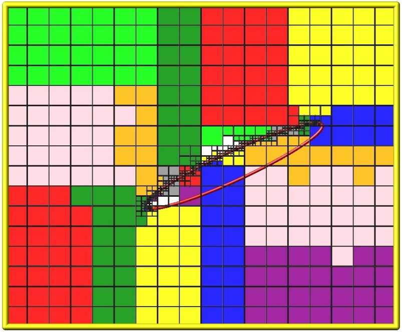
National Nuclear Security Administration

How SPARTA works in parallel

- 3 kinds of data: **particles, grid cells, surface elements**
  - hierarchical Cartesian grid with cells cut/split by surfs
  - grid cells (and their particles) are load balanced (RCB)
  - surface elements are not (yet) distributed



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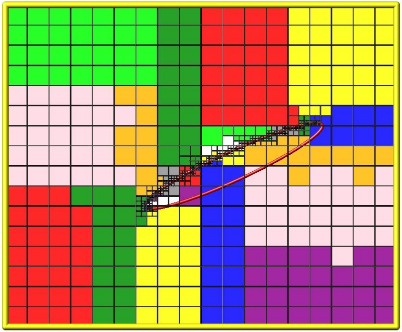
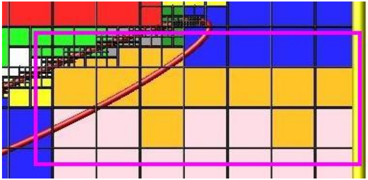




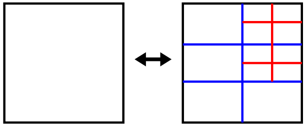
- Each proc: **clump** of child cells + **ghost cells** within cutoff
- **One-pass communication** per step, if cutoff long enough

Interesting features, current and future

- Adaptive gridding
- Run on GPU, KNL via Kokkos
- Code extensibility
- **Distributed surfaces**

Adaptive gridding

- **Hierarchical** grid
  - top-level is single grid cell = simulation box
  - each parent cell has variable Nx by Ny by Nz child cells
  - recurse as many levels as desired (64-bit cell IDs)
  - oct-tree is 2x2x2 case, up to 15 levels
- Each child or parent cell considered **independently**



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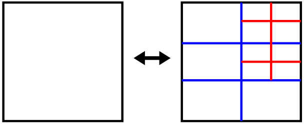
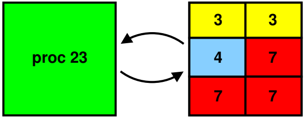


- **Refinement/coarsening criteria**:
  - any per-grid value, current or time-averaged
  - geometric: nearness to upwind surface elements
  - flow: number of particles in cell,
    mean-free-path $= \lambda = \{\sqrt{2}\pi D_{\mathrm{ref}}^2 n (T_{\mathrm{ref}}/T)^{\omega-1/2}\}^{-1}$

Parallel implementation

- **Refinement** is a **local** operation
  - proc that owns a child cell can decide to refine, create new cells
  - all procs can do this without communication
- **Coarsening** may **not be local** operation
  - if one proc owns all children, then local
  - if multiple procs own children, communication needed



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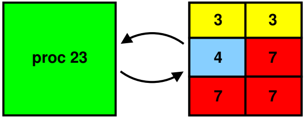
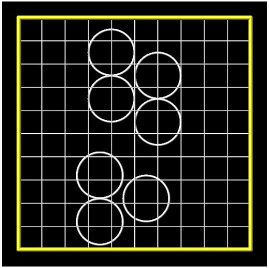
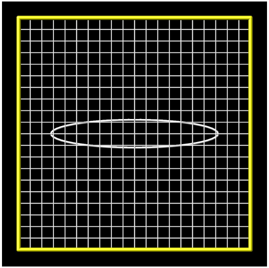
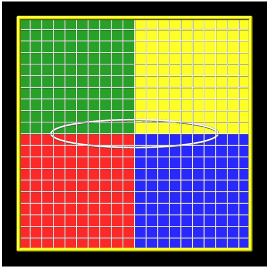


- Use **rendezvous** algorithm for non-local coarsening
  - owner of each child may not know who owns other children
  - everyone knows rendezvous proc, send child info to it
- **Rendezvous processor**
  - owner of parent cell, assigned in round-robin fashion
  - gathers info from all children, decides whether to coarsen
  - communicates result to all procs owning child cells

Simple 2d examples

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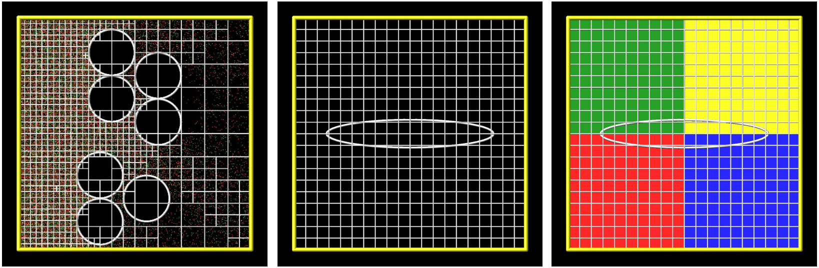
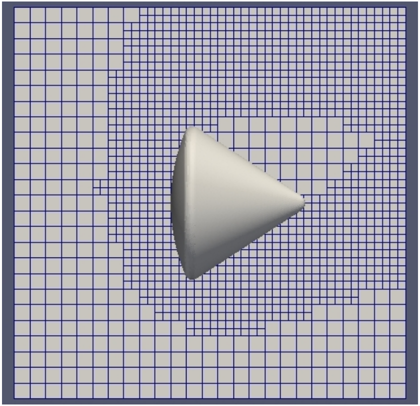


For moving surfaces:

- remove particles from any cell cut by element
- assume move is slow enough to allow particles to re-equilibrate

3d flow around Apollo capsule

- 74 million particles, initial coarse grid $= 25^3 = 16\text{K}$ cells



- Final 5-level refined grid $= 6.5$ million child cells
- Uniform grid at fully refined scale $= 800^3 = 512\text{M}$ cells

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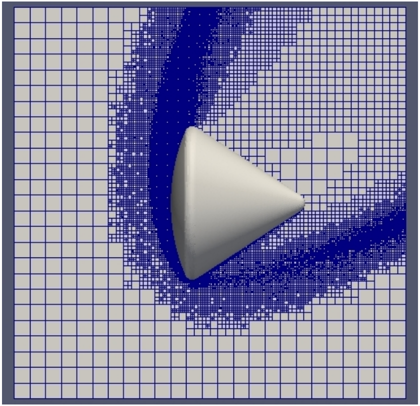

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- Work by Stan Moore and Dan Ibanez
- Kokkos: **https://github.com/kokkos**
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- Two major components:
  1. Data access abstraction via **Kokkos arrays**
     - optimal layout & access pattern for each device
     - CPU, GPU, KNL, etc
  2. **Parallel dispatch** of small chunks of work
     - auto-mapped onto back-end languages
     - CUDA, OpenMP, etc

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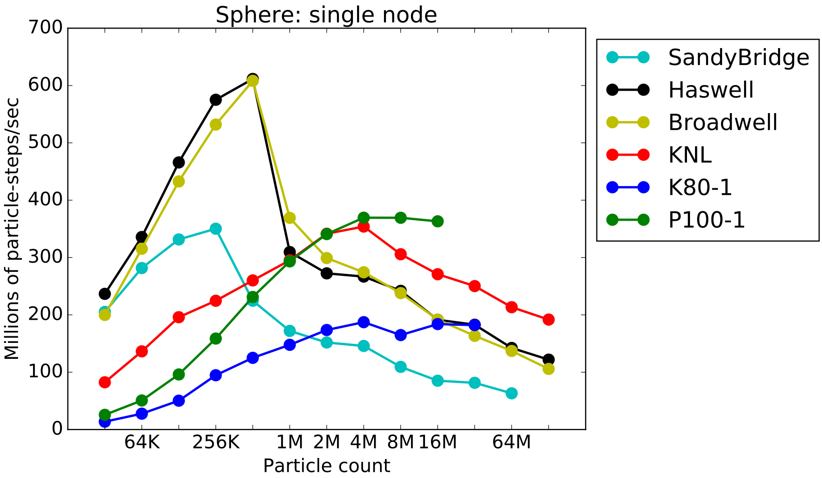
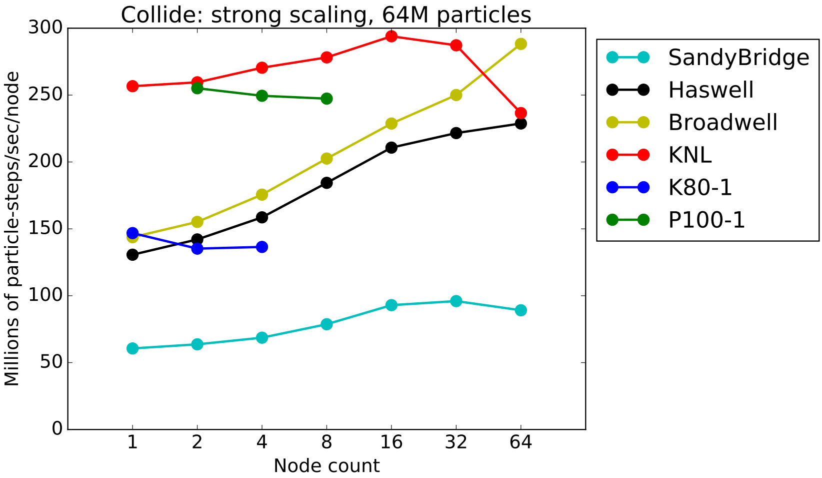
- Incremental rewrite of SPARTA **kernels** so they:
  - use Kokkos data structures, fine granularity, thread-safe
  - status: move, sort, collide, **hierarchical grid, surfs**
  - not yet: reactions, many diagnostics, BC, etc

Single-node SPARTA performance on CPU, GPU, KNL



Strong-scaling SPARTA performance on CPU, GPU, KNL



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- Virtual parent class defines interface to a **capability**
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Examples:

- collision & reaction models = VSS, VHS, QK, TCE, hybrid
- surface collision models = specular, diffuse, piston, vanish
- surface reaction models = global, list of reactions/probabilities
- **diagnostics** (16) = various per-particle, per-grid, per-surf
- **fixes** (14) (operate while timestepping) = particle emission, time averaging, load-balancing, move surfs, etc
- fixes can define additional per-particle attributes: **ambipolar**, polyatomic vibrational **energy levels**

SPARTA can be used as a library

At least **two purposes**:

- Use SPARTA as a tool in a higher-level **workflow**
  - can invoke multiple instances of SPARTA
- Enable **multi-physics** or **multi-scale** models
  - couple to continuum or molecular collision models

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Software details:

- C-style interface, callable from C++/C/Fortran/**Python**
- Parallel python via mpi4py
- Lib interface is easy to extend:
  - add functions to library.cpp/h
  - add wrapper methods to sparta.py for Python
- Umbrella code/script can invoke SPARTA and another code, pass info between them

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Caveat: not solving the hard coupling problem, just software issue

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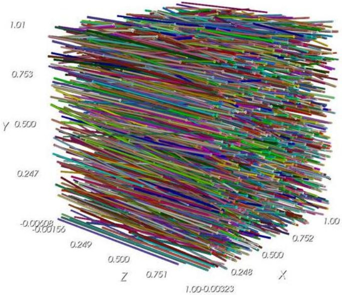

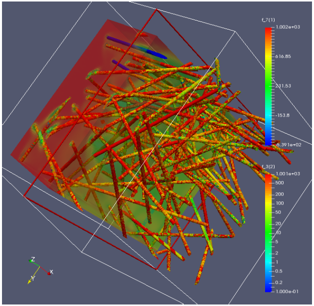

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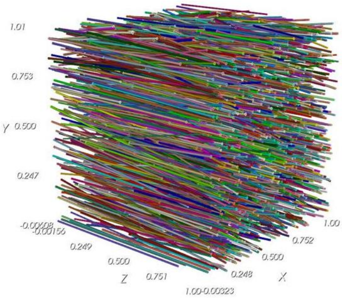

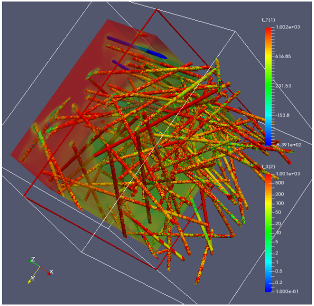

- Currently each proc stores all surfs:
  - easier to not worry when a surf overlaps many cells/procs
- One surf = $\sim$80 bytes + tallies $\Rightarrow$ **100s GBs**
- **New option** for proc to only store surfs in owned+ghost cells

Complicating factors

- Load-balancing
  - surfs now have to **migrate** with cells/particles
- Per-surf-element **statistics**
  - currenty tallying is via MPI_Allreduce()
  - will need to do something more clever
- Surface **erosion**:
  - how to maintain **topology**
  - more careful nearby particle deletion/creation
- Do we need to store per-surf-element **state** ?
  - multiple procs may contribute to one element's state
  - how to insure state is **up-to-date**

Thanks and links

- **Funding** support: DOE/NNSA ASC and ATDM programs

- **http://sparta.sandia.gov**
- SPARTA short course:
  http://sparta.sandia.gov/**tutorials.html**

- Stan Moore and Dan Ibanez (Sandia): Kokkos work
- **https://github.com/kokkos**

- Looking to **collaborate** on new ideas for SPARTA
- magalli@sandia.gov, sjplimp@sandia.gov