Parallel Simulation of Dendritic Growth On Unstructured Grids

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Outline

1. What and why?
2. Specialized Parallelization
3. Stencilized Parallelization
What and why?

Specialized Parallelization

Stencilized Parallelization

Outlook
Simulation of Dendritic Growth in Al/Cu

- Microscope
  - two classes of models:
    1. cellular automata (our approach)
    2. phase field method
      (Peta-scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer)
  - meshfree (no regular grid)

- Simulation
**Simulation Model**

- **black**: solid cells
- **green**: liquid cells
- **squares**: particles on phase boundary
Outlook

1. What and why?

2. Specialized Parallelization

3. Stencilized Parallelization
1. decompose graph via ParMETIS
2. loop
   1. sync ghostzones
   2. update
   3. (output)
Communication Graph

- 10^6 cells, 10 MPI processes
- 74k ghost cells
- 2 GB/step
10^6 cells, 100 MPI processes
475k ghost cells
11 GB/step
Outlook

1. What and why?

2. Specialized Parallelization

3. Stencilized Parallelization
Stencilization

- superimpose grid on irregular graph
- place cells into container cells
- physically equivalent
  - reuse existing library: LibGeoDecomp
    - overlapping comm. & calc.
    - hybrid parallelization
Stencilization

- superimpose grid on irregular graph
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- testbed: 28 IBM LS21 blades (Opteron dual-cores)
- 10 Gb InfiniBand
Overlapping Communication and Calculation

- Myth #1: It’s as easy as calling MPI_Isend()
- Myth #2: It’s not possible at all

1. MPI_Isend()
2. loop
   1. MPI_Test()
   2. work()
3. MPI_Wait()
Myth #1: It’s as easy as calling MPI_Isend()
Myth #2: It’s not possible at all

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Overlapping Micro Benchmark

- 16, overlap, send
- 64, overlap, send

Open MPI + InfiniBand
Conclusion

- communication-bound model
- *stencilization* surprisingly efficient
  - reduces number of neighbors
  - but model changes may be substantial
- use MPI+OpenMP to reduce memory traffic
- asynchronous communication by repeatedly poking MPI

LibGeoDecomp
Self-Adapting Stencil Codes for the Grid

http://www.libgeodecomp.org
<table>
<thead>
<tr>
<th>What and why?</th>
<th>Specialized Parallelization</th>
<th>Stencilized Parallelization</th>
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<tbody>
<tr>
<td>Backup</td>
<td></td>
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Improving Data Locality for Communication
Efficient Memory Layout

Original Layout

- SimSpace
- SimObject
  - position
  - state
  - concentration
- Cell
  - ID
  - neighborIDs
- Particle
  - IDsource
  - IDtarget
  - velocity

Optimized Layout

- Grid
- ContainerCell
  - position
  - dimensions
- Cell
  - ID
  - neighborIDs
- Particle
  - IDsource
  - IDtarget
  - velocity

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Simulation of Dendritic Growth in Al/Cu

Microscope
- model courtesy of
  - Department of Metallic Materials, FSU Jena, Germany
- name derived from greek δενδρον (dendron)
- not supercooled

Simulation