Hybrid OpenMP/MPI with Cactus and Carpet

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OpenMP Parallelisation: Quick Facts

- OpenMP can parallelise within one node only (requires shared memory)
- Saves memory (no ghost zones required); reduces cache pollution
- Can improve scaling (since fewer MPI processes for same number of cores)
- OpenMP directives are ignored by default (are safe to add to existing code)
- OpenMP is supported almost everywhere

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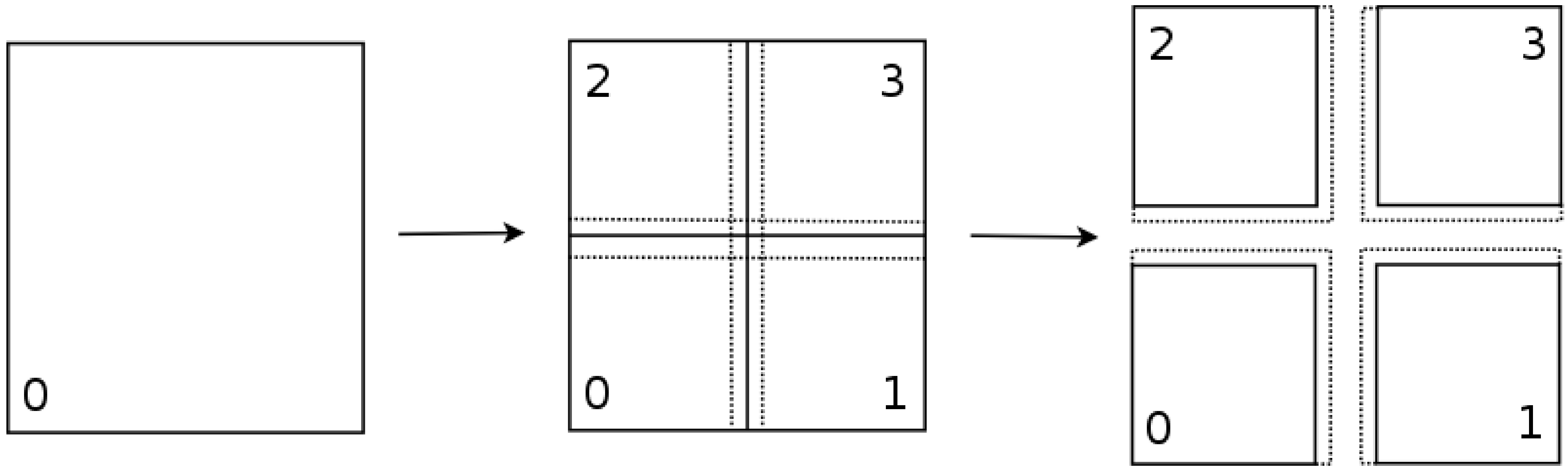
Background: MPI Parallelisation

- Decompose domain, one subdomain for each process
- Introduces ghost zones, creating memory overhead
- Requires synchronising after modifying grid functions



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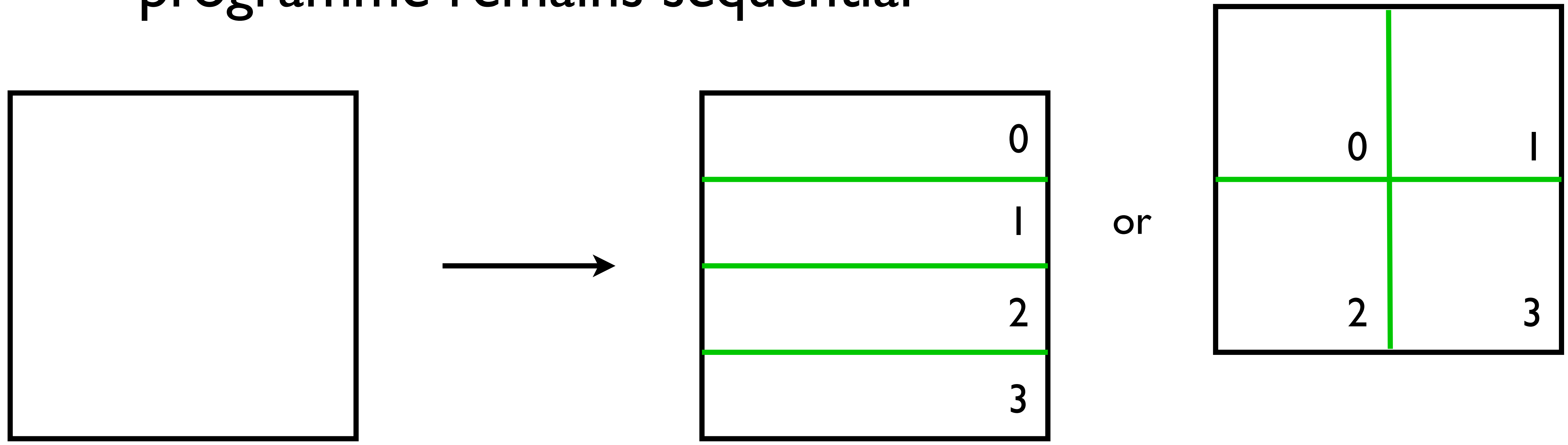
OpenMP Parallelisation

- Threads share same memory, work on same arrays
- No ghost zones, no memory overhead
- No synchronisation required
- Usually, only loops are parallelised, remainder of programme remains sequential



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Sample Calculation: Ghost Zone Memory Overhead

- Assume 20^3 grid points per process, 3 ghost zones (4th order with advection)
  - evolved points: $20^3 = 8{,}000$
  - overall points: $(20+2\cdot3)^3 = 17{,}576$
  - ghost zone overhead: 120% (factor 2.2)
- (Lesson: "3" is a large number if it is found in an exponent...)

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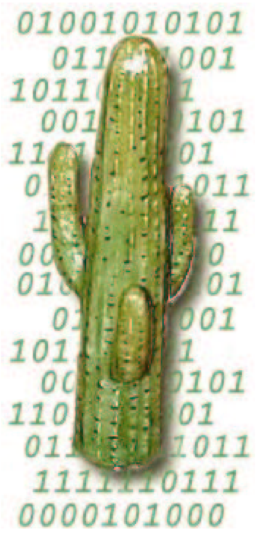
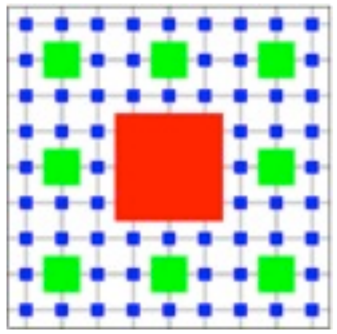
Current State



- Most of Cactus, PUGH, Carpet parallelised via OpenMP (but not everything fully optimised yet)
  - Note: Can parallelise incrementally by looking at timer output, working on slowest routines
- New codes (CTGamma, McLachlan, etc.) fully parallelised
- Hand-written Fortran codes (CCATIE, Whisky) not yet parallel (tedious!)
- "Serial thorns" in Einstein Toolkit (TwoPunctures, AHFinderDirect) partly parallelised



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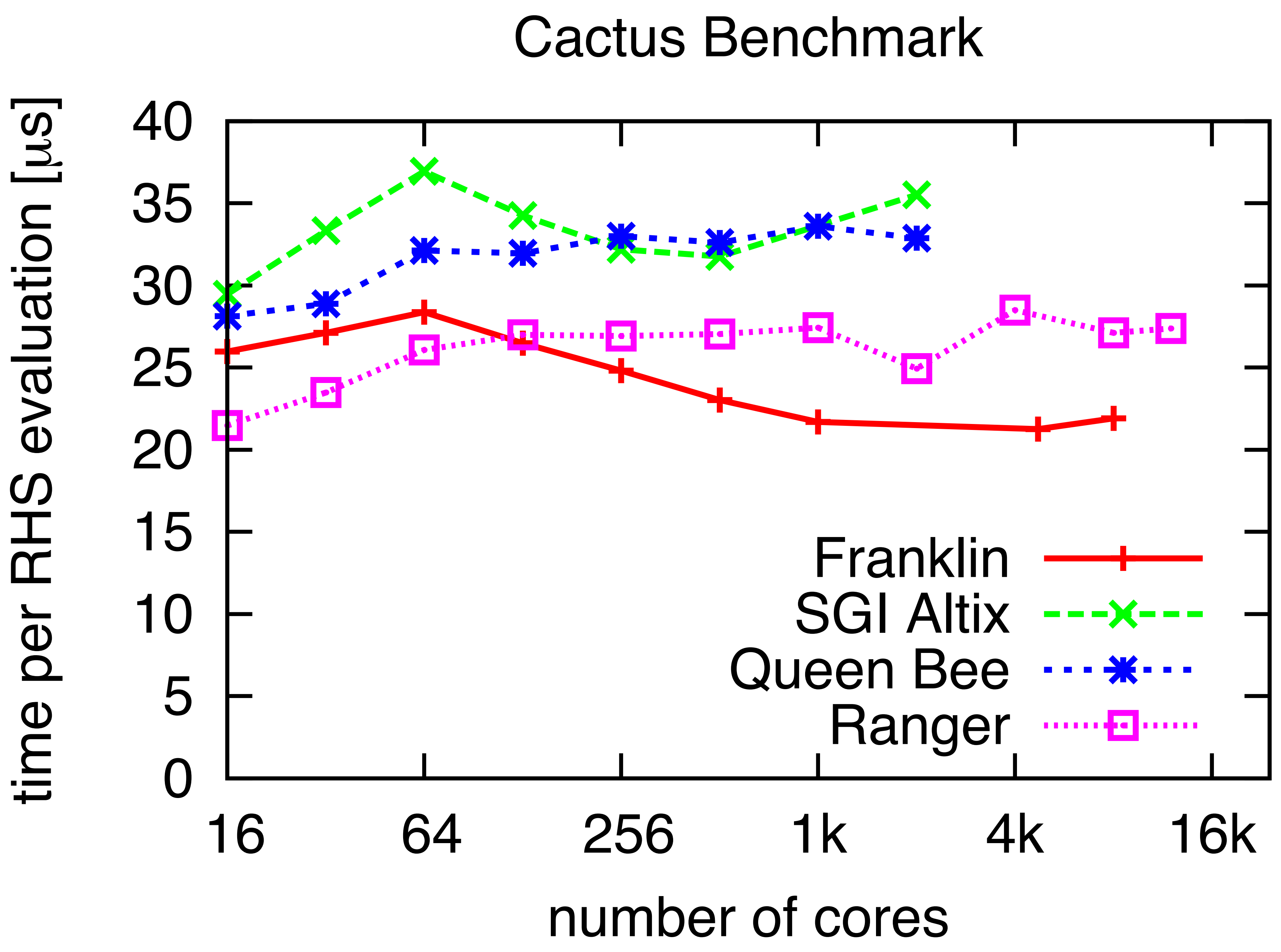
Benchmark (Scaling)



- Setup:
  Carpet, McLachlan,
  9 AMR levels
- 25^3 per core,
  3 ghost zones,
  weak scaling
- infrastructure scales well (except regridding)
- uses OpenMP to improve scalability

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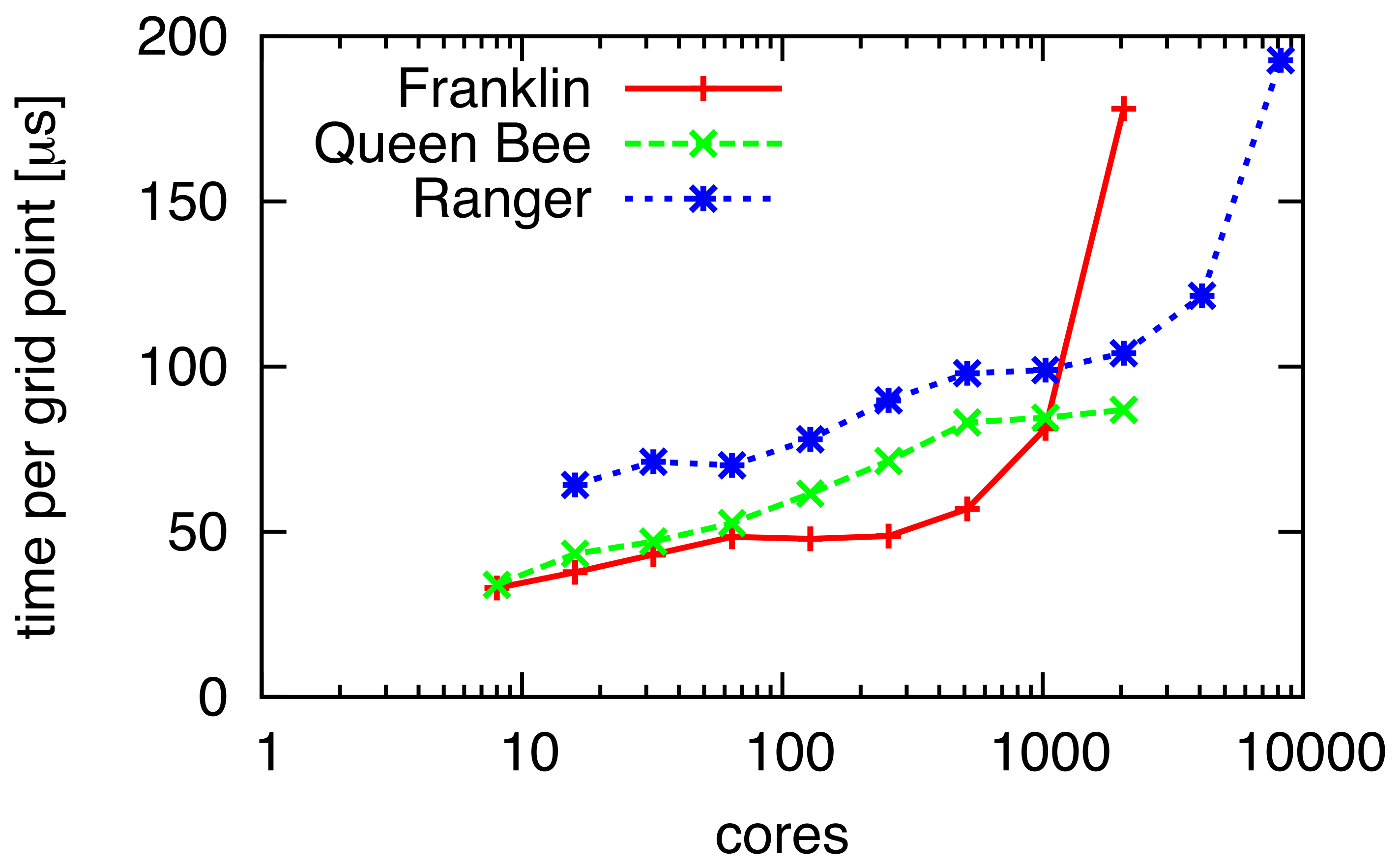
Improved Scaling via OpenMP

McLachlan/Carpet AMR Scaling



[Outdated results, March 2008]

- Note: these are outdated weak scaling results, demonstrating how scaling breaks down
- different #OpenMP threads:
    Franklin: 1
    Queen Bee: 8
    Ranger: 4
- scaling breakdown depends on #MPI processes, not on #cores
- Using N threads improve scaling by a factor of N

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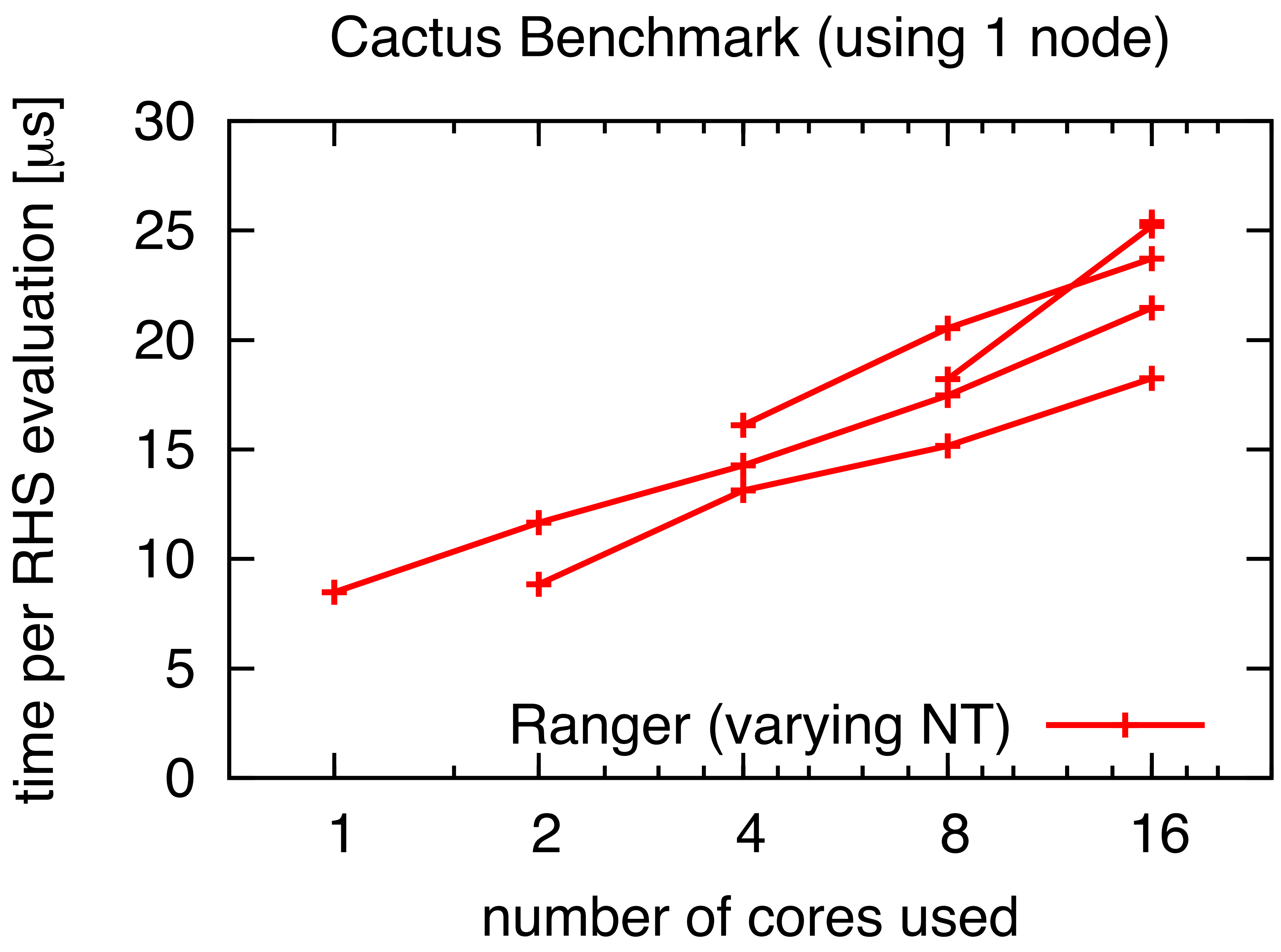
Benchmark (Single Node)



- Varying #cores used, #MPI processes, #OpenMP threads
- ideal scaling would be horizontal line
- using more cores reduces per-core performance
- using OpenMP changes performance

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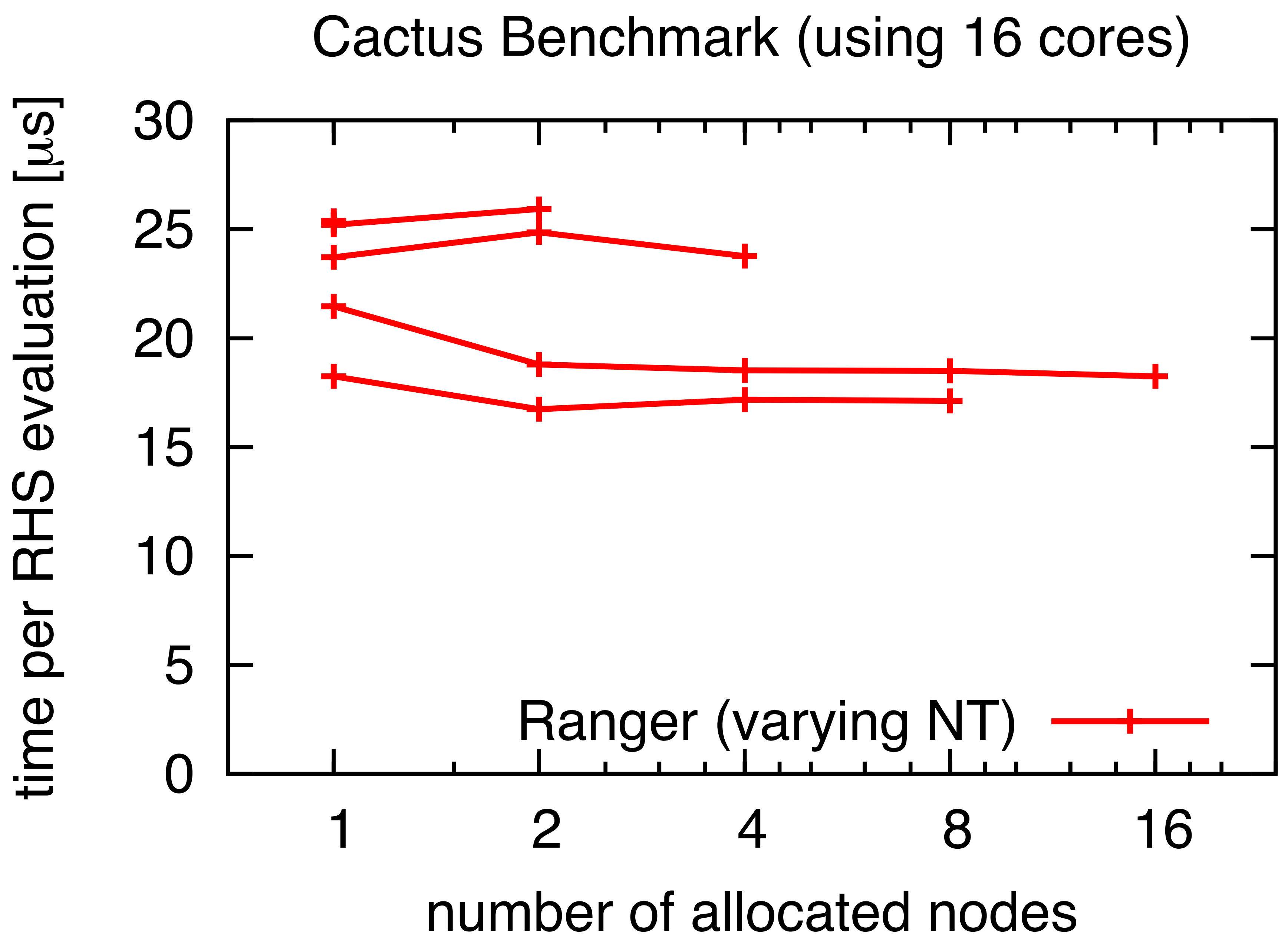
Benchmark (shared memory vs. interconnect)



- Varying #nodes used, #MPI processes, #OpenMP threads
- ideal scaling would be horizontal line
- using more nodes does not influence performance much
- using OpenMP changes performance

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Future Benchmark Work

- Previous slides examine only wall time
- Need more low-level information:
  - cycles, instructions, cache misses, memory bandwidth thread/MPI wait times, etc.
  - compare different architectures, compilers, build options (>30% unexplained difference between different systems)
- Given allocation shortages, 30% difference is huge

OpenMP Support in Tools

- Kranc: automated code generation <http://numrel.aei.mpg.de/Research/Kranc/>
  - Kranc generated code is fully parallelised with OpenMP
- SimFactory: simulation management <http://www.cct.lsu.edu/~eschnett/SimFactory/>
  - Cactus configurations built by SimFactory use OpenMP compiler options by default
  - Simulations started via SimFactory can use OpenMP easily (--num-threads=N)

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LoopControl

- Generic mechanism to loop over grid functions, can replace nested for/do loops
  - automatically tiles loops (can improve cache efficiency)
  - automatically parallelises via OpenMP
  - LoopControl keeps performance statistics, and can optimise its tiling/parallelisation parameters at run time

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LoopControl Example

Original:

```
#pragma omp parallel for
for (int k=1; k<cctk_lsh[2]-1; k++) {
  for (int j=1; j<cctk_lsh[1]-1; j++) {
    for (int i=1; i<cctk_lsh[0]-1; i++) {
```

with LoopControl:

```
#include <loopcontrol.h>
#pragma omp parallel
LC_LOOP3 (wavetoy, i,j,k,
          1,1,1,
          cctk_lsh[0]-1,cctk_lsh[1]-1,cctk_lsh[2]-1,
          cctk_lsh[0],cctk_lsh[1],cctk_lsh[2])
{
```

- LC_LOOP3 macro hides complexity
- Perform loop optimisations (tiling, different OpenMP topologies)
- Could introduce other optimisations later, without changing macro calls

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Programming with OpenMP (Not A Tutorial)

- With OpenMP, typically individual loops are parallelised, leaving other code unchanged
- Loops have OpenMP directives added, e.g.

```
#pragma omp parallel for
```

- Need to use special compiler flag (e.g. -openmp) to enable directives (otherwise they are ignored)
- See <http://www.openmp.org/>; many tutorials on the web

OpenMP Concepts

- To be parallelised, the individual iterations of a loop must be independent:
  - the order of execution must not matter
  - different iterations must not access the same variables
- Good examples: RHS evaluation, con2prim
- Not parallel: Gauss-Seidel iteration, performing I/O

OpenMP Fortran Example: Whisky, con2prim

```
!$omp parallel do private (epsnegative, det,
         uxx,uxy,uxz,uyy,uyz,uzz, psi4pt, enthalpy)
do k = 1, nz
  do j = 1, ny
    do i = 1, nx
```

good: only need to annotate 3D loops

bad: need to list all temporary variables used in the loop

C, C++: can declare variables inside loop (much simpler)

```
!$omp critical
         call CCTK_WARN(1,'Con2Prim: stopping the code.')
!$omp end critical
```

can do I/O in parallel loop if OpenMP is told about it

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Private Variables, Reduction Operations

- If a loop uses temporary variables, they either need to be declared inside the loop, or need to be declared as <u>private</u>
  - In other words: you need to tell OpenMP about it, then you're fine
- Likewise, if a <u>reduction</u> (e.g. sum) is performed, OpenMP needs to be told
- Some loops just cannot be parallelised; if you do, you may silently sometimes receive wrong results