Center for Scalable Application Development Software: Application Engagement

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Application Engagement

- Workshops (2 out of 4) for outreach
  - Leadership Class Machines, Applications, and Performance
  - Scientific Data Analysis and Visualization for Petascale Computing

- Other application engagement
  - continued interactions with workshop participants
  - focused engagement with specific application groups

Workshop on Leadership Class Machines, Applications, and Performance

- Goal: Jumpstart productive application use of DOE’s large-scale facilities at ANL, ORNL, and NERSC
- Target audience
  – code developers; not necessarily P.I.’s
  – from DOE SciDAC and INCITE programs
- Content (presented by 12 speakers)
  – leadership machine architectures
  – programming at scale for performance
  – tools for understanding code behavior
  – I/O and visualization
  – hands-on sessions (time for hacking, with sysadmins available)

Attendees and Their Projects

- 2008: 25 attendees
  - 12 from projects with INCITE awards
  - 15 from other SciDAC projects
- Wide range of application areas, e.g.:
  - climate INCITE
  - FACETS SciDAC (fusion)
  - CSCAPES SciDAC
  - COMPASS SciDAC (particle accelerator modeling) also INCITE
  - biofuels INCITE
  - combustion in gas turbines INCITE

Interactions Born at the Workshops

- Revised approach to parallel I/O for sparse matrix data structures, used in part of UNEDF SciDAC. Interactions continued at recent Nuclear Physics Exascale meeting
- Alternate file format and parallel I/O strategy for PHASTA. Continued at ALCF workshop in January.
- Turbulent flow project for Center for Turbulence Research at Stanford. I/O strategies on Franklin (NERSC machine). Ported code to BG/P. Continued interactions with ALCF staff
- Worked with CERFACS on problem decomposition; student visited Argonne for further optimization work.
- Formed collaboration with NERSC on HDF5 issues.
- Worked closely over the year with GFMC part of UNEDF SciDAC.

Lasting relationships formed at Snowbird workshops

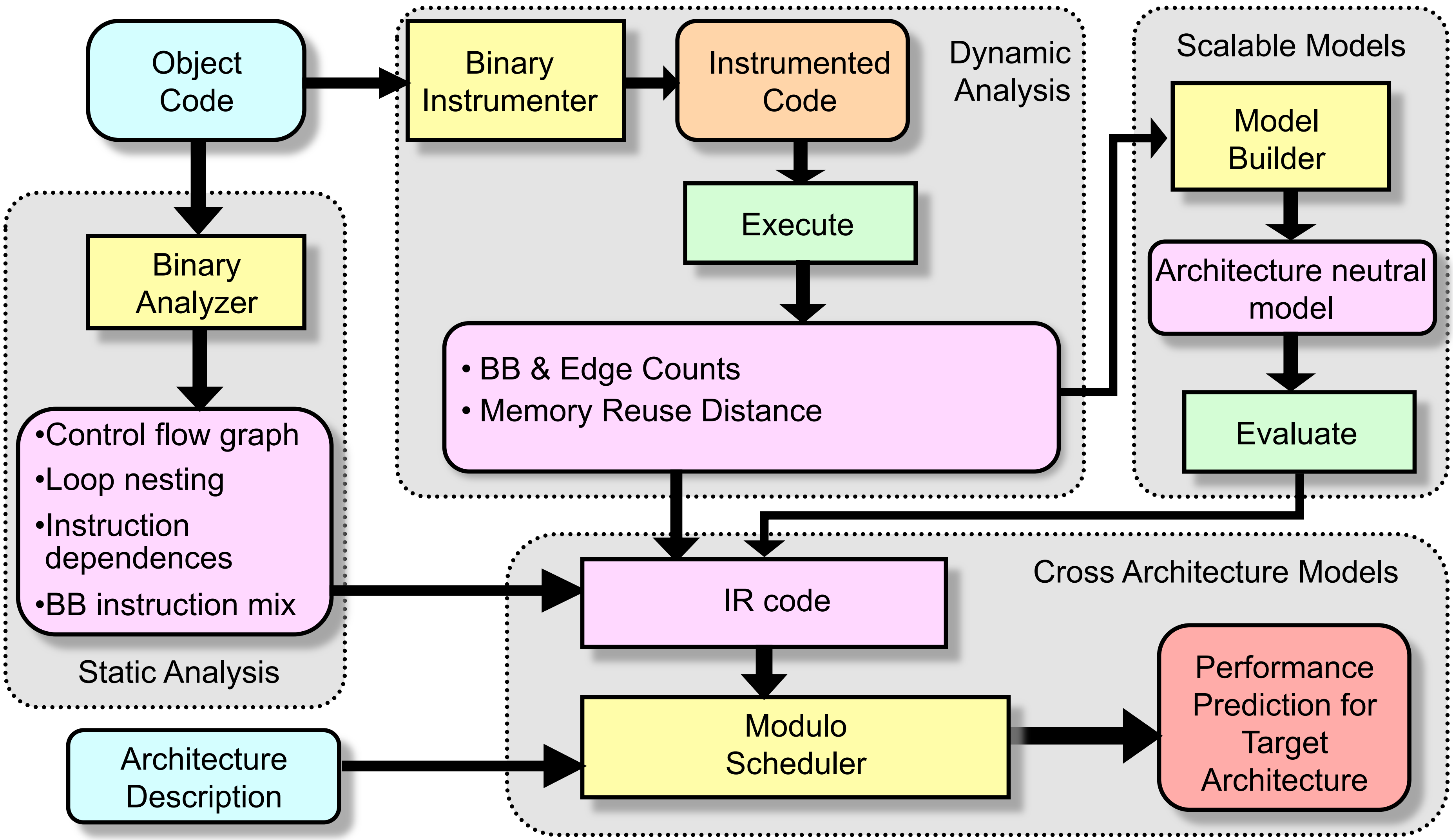
Focused Engagement Activities

- Need representative applications to drive compilers/tools research
- CScADS collaborates in PERI Tiger Teams
  - PERI Tiger Teams engage CScADS with applications
  - CScADS extends PERI Tiger Team efforts
  - develop software and methods to help application teams
    - GTC: particle-in-cell simulation of turbulent plasma in a tokamak
    - FLASH: block structured AMR to simulate astrophysical flashes
    - S3D: direct numerical simulation of combustion using dense arrays

The Challenge of Application Tuning

- Performance measurement tools identify
  - sections of code that execute inefficiently
  - loops that incur a high fraction of a particular hardware event
- Knowing where cache misses occur is seldom enough
  - data reuse is not a local phenomenon
- Assess tuning opportunities through modeling
  - identify performance bottlenecks due to application characteristics
    - instruction level parallelism, data reuse patterns, data layout
  - provide insight into code transformations for improving performance
    - PERI aims to provide guidance for next generation procurements
    - CScADS aims to help improve application performance
  - understand performance impact for a target architecture
    - understand mismatch between application and architecture
    - impact of ILP depends on machine width, execution unit types

Modeling Toolkit Design Overview



Understanding Data Reuse

Identify data reuse patterns using reuse distance

- Characterize reuse patterns by a tuple of scopes
  – source, destination, carrying scopes
- Understand not only where cache misses occur
  – identify where data has been previously accessed
  – identify which algorithmic loop is driving the reuse
    - important for understanding how to improve the reuse

```
do kz=1,mzbig
   wz=real(kz)/real(mzbig)
   zdum=zetamin+deltaz*(real(k-1)+wz)
   do i=idiag1,idiag2
      ii=igrid(i)
      do j=1,mtdiag
         …
         phiflux(kz+(k-1)*mzbig,j,i)= …
      enddo
   enddo
enddo
```

GTC example

–spatial reuse

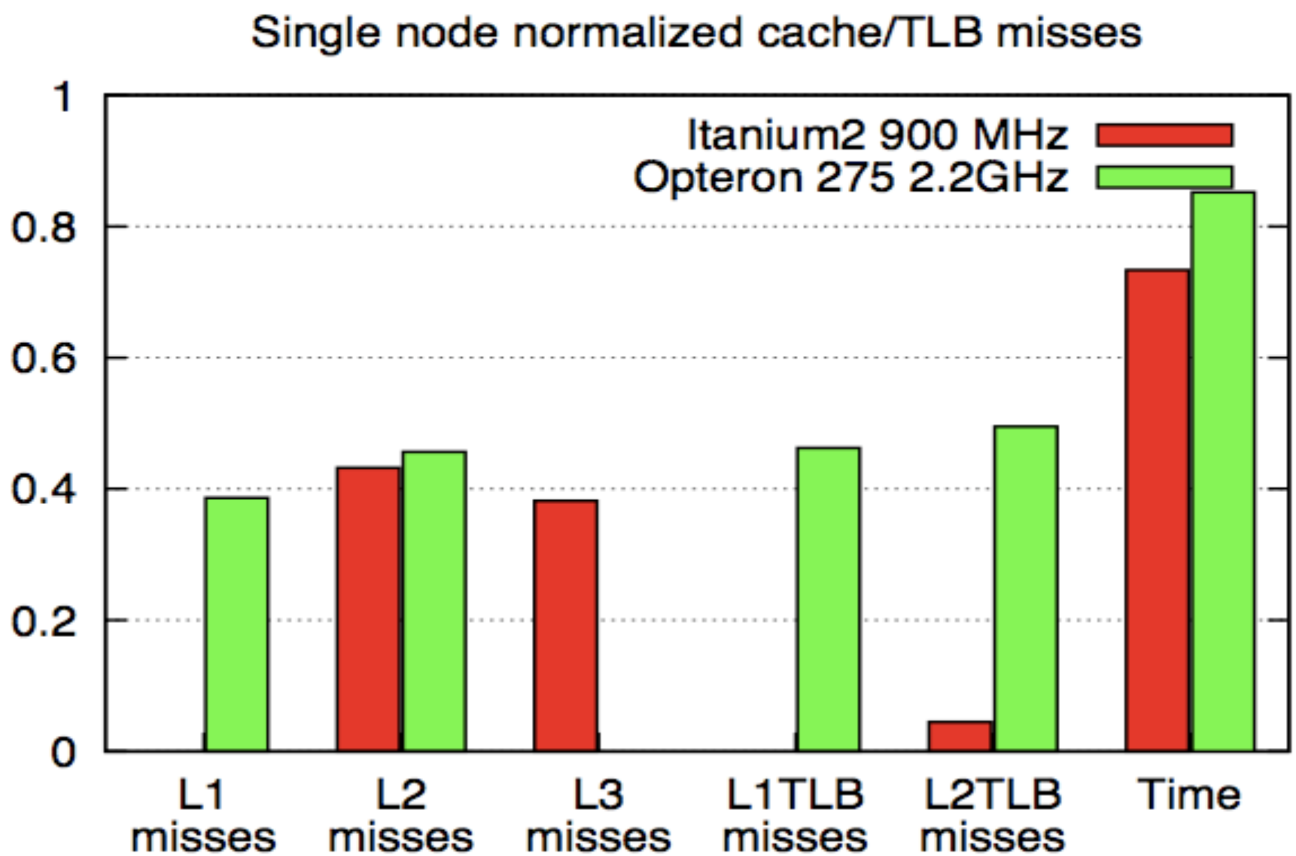
Missed Opportunities for Spatial Locality

- Problem: inefficient use of caches
  - long temporal or spatial data reuse
    - captured by memory reuse distance
  - unused data in cache lines
    - data fetched in blocks; some words never accessed
    - *fragmentation factor* = $\dfrac{\textbf{\textit{data fetched but never accessed}}}{\textbf{\textit{total fetched data}}}$
- Approach
  - compute fragmentation factors for references
    - use static analysis to understand access stride and fraction of data never accessed
  - report misses due to data fragmentation at each level

Application Engagement: GTC

- GTS: simulates turbulent plasma in tokamak reactors
  - 3D particle-in-cell code; 1D decomposition along toroidal direction
    - charge: deposit charge from particles to grid points
    - solve: compute the electrostatic potential and field on grid points
    - push: compute the force on each particle from nearby grid points
- Used measurement and modeling tools developed at Rice with CScADS support to pinpoint performance losses
  - poor spatial locality due to vector of structures representation for ions
  - unrealized opportunities for temporal reuse between loops over ions
- Improving node performance
  - manually transform to structure of vectors
  - manually apply fusion and blocking to improve temporal reuse
  - transmit improvements back to GTC/GTS code teams

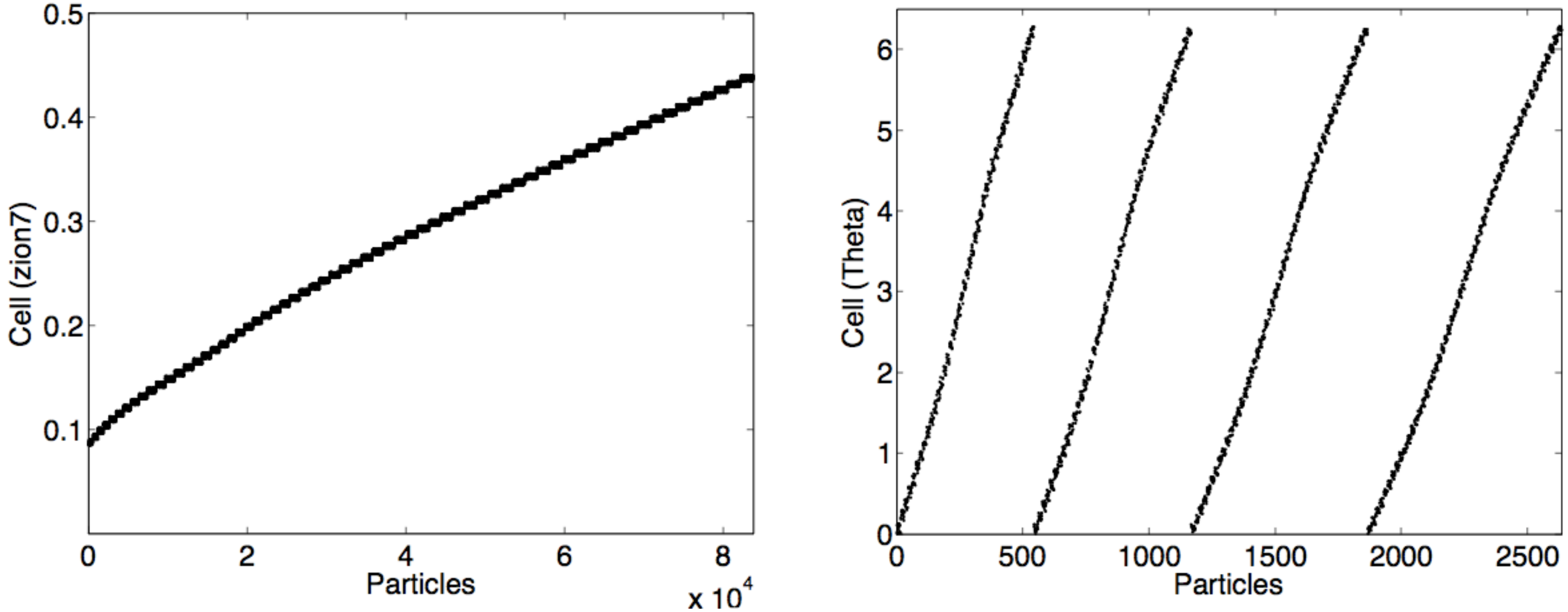
GTS: Node Performance Improvements



- Metrics normalized to measurements of original code
- Lower is better

GTS: Locality Degrades as Ions Swirl

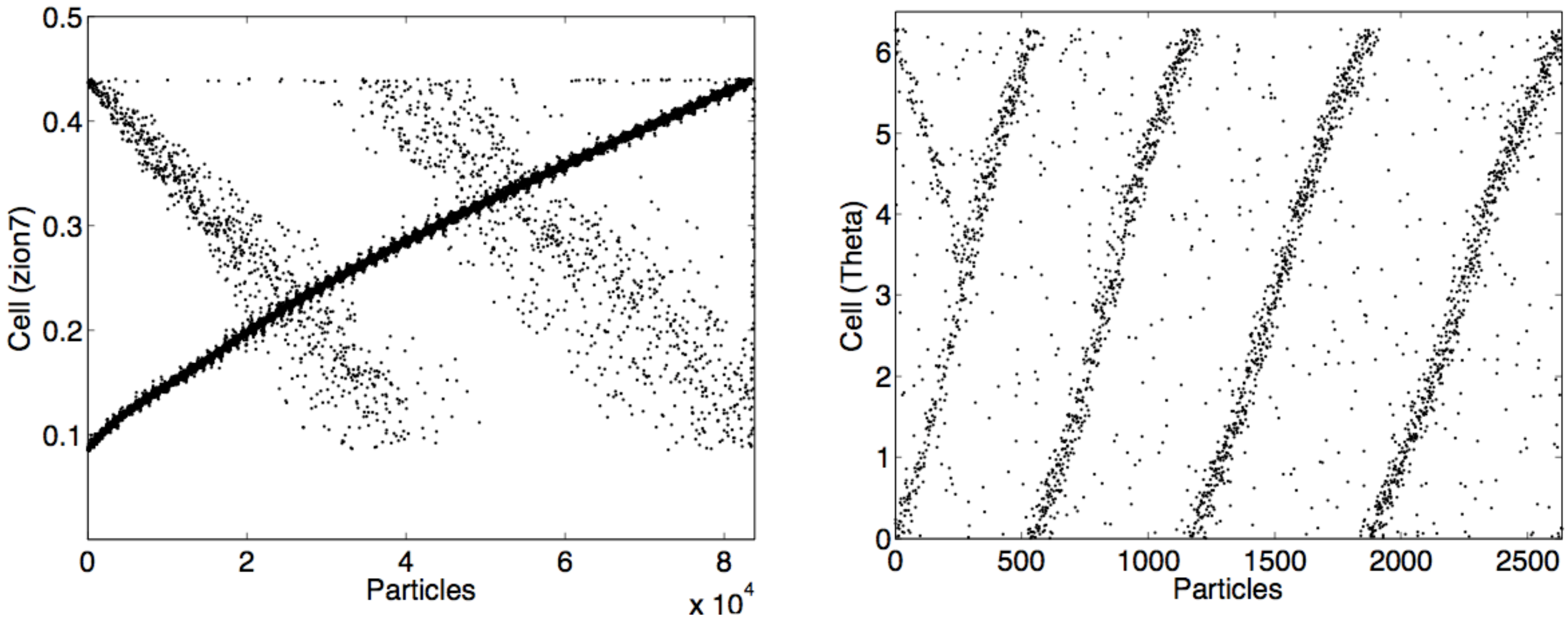
- Locality is best when particles are sorted in cell order
  - —potential computation uses cell data only
  - —charge deposition and particle pushing involve interactions between particles and cells
- Initially particles are uniformly distributed in cell order



Time step 0

GTS: Locality Degrades as Ions Swirl

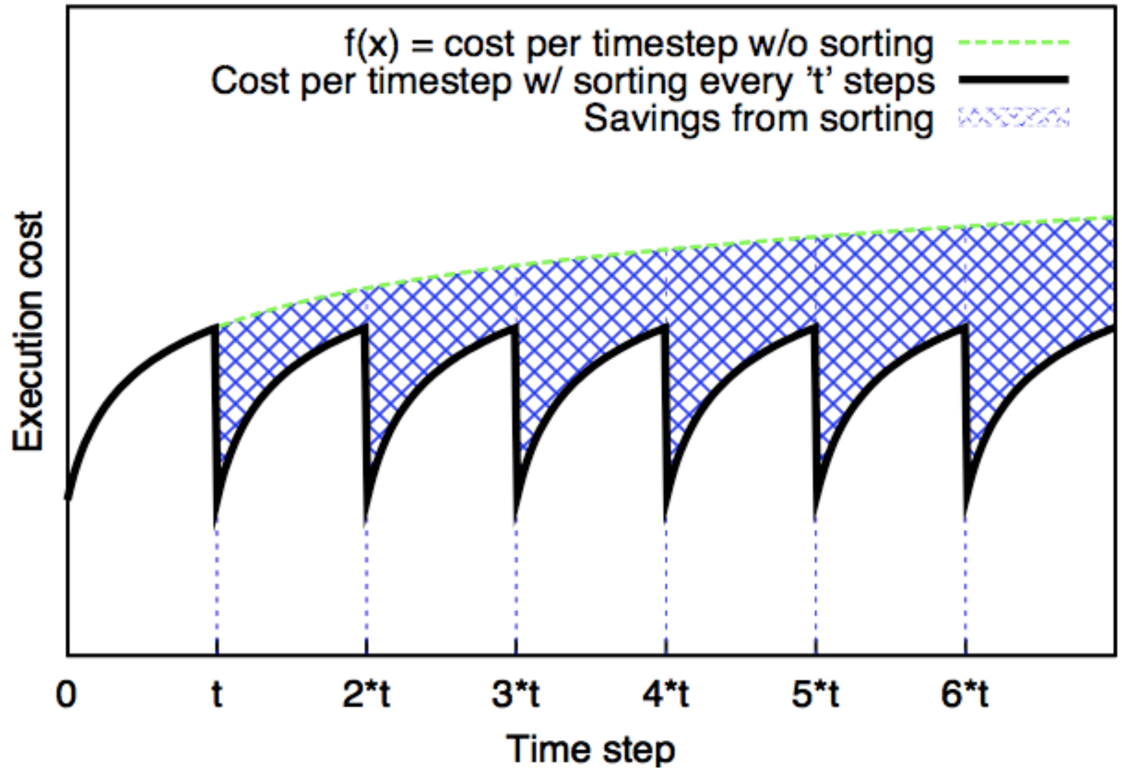
- Locality is best when particles are sorted in cell order
  - —potential computation uses cell data only
  - —charge deposition and particle pushing involve interactions between particles and cells
- <u>Over time, the particle distribution diverges from cell order</u>



Time step 20

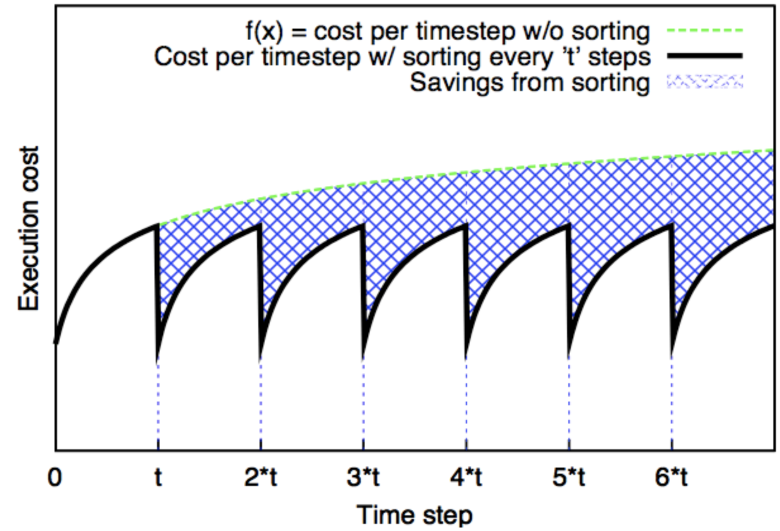
GTS: Potential Improvement from Reordering

- Locality degrades gradually at run-time
- Assumptions:
  - —periodic particle reordering restores locality and performance
  - —performance degrades at similar rate after each sorting step



GTS: Compute Optimal Sorting Interval

- Notations
  - —f(x) = time step cost function
  - —C = cost of sorting
  - —G(t) = gain from sorting every t time steps
- Find t that maximizes G(t) over N steps



$$G(t) = \sum_{k=1}^{\frac{N}{t}-1} \left(\int_{kt}^{(k+1)t} f(x)\,dx - \int_0^t f(x)\,dx - C \right)$$

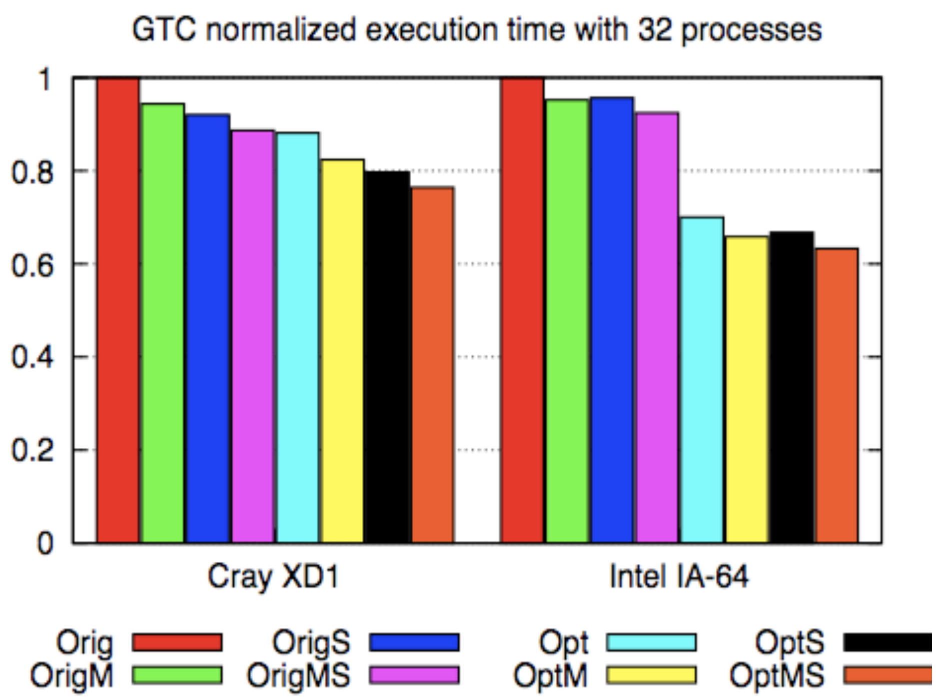
terms constant in t

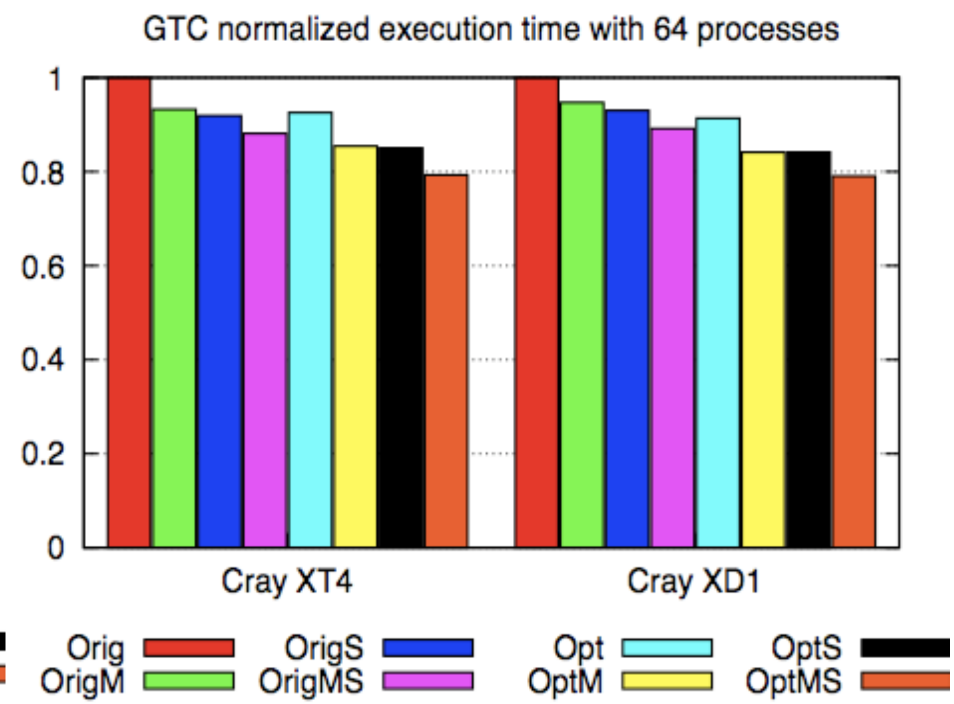
$$G(t) = \boxed{\int_0^N f(x)\,dx} - \frac{N}{t}\int_0^t f(x)\,dx - \frac{N}{t}C + \boxed{C}$$

- Find t that minimizes $h(t) = \frac{1}{t}\left(\int_0^t f(x)\,dx + C \right)$

- h(t) = average time step cost with sorting

Parallel Performance Results



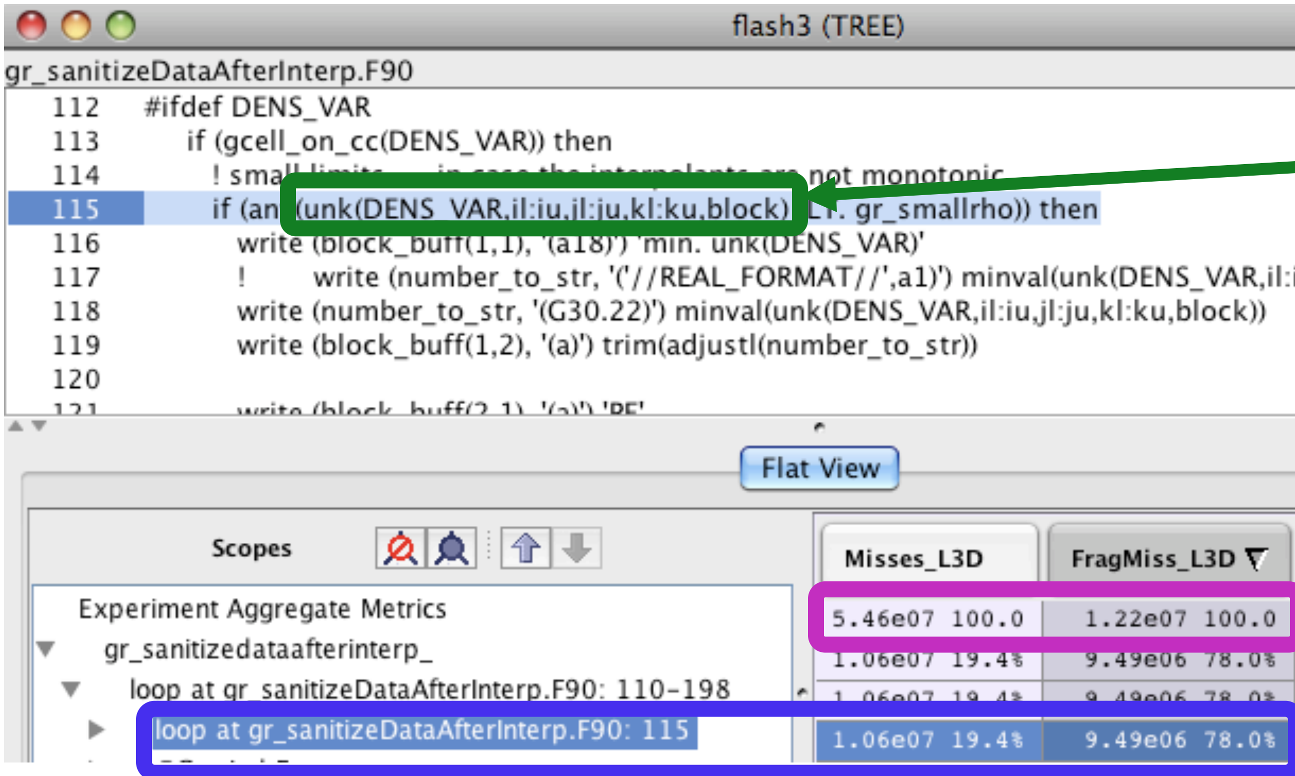


- Combined optimizations reduce GTS execution time by
  - —37% on Itanium2 cluster
  - —21% on Cray XT and Cray XD1

Application Engagement: FLASH

FLASH suffers from poor spatial locality due to data layout

(values predicted for Sedov test case)



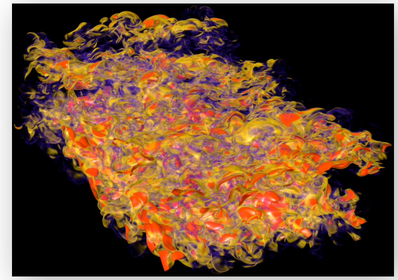
Array `unk` – main data structure holding cell centered data for PARAMESH – has variable index on innermost dimension.

- Total L3 miss count
- L3 cache misses due to fragmentation of data in cache lines: 22% of total

array statement at line 115 accounts for 78% of fragmentation misses

Application Engagement: S3D

- Direct numerical simulation (DNS) of turbulent combustion
  - state-of-the-art code developed at CRF/Sandia
    - PI: Jaqueline H. Chen, SNL
  - 2007/2008 INCITE awards at NCCS
  - pioneering application for 250TF Jaguar system



- Extend performance analysis work of PERI Tiger team
  - use HPCToolkit to locate single-core performance bottlenecks
    - compiler inserted array copies
    - streaming calculations with low data reuse
    - loop nests with recurrences
  - identified opportunities for compiler-based improvement
  - enhanced LoopTool to address S3D's needs
  - improved loop nests with LoopTool's semi-automatic transforms
    - transformed code is now part of S3D's source base
  - used HPCToolkit to assess multicore scaling issues

J H Chen et al 2009 Computational Science and Discovery 2 015001 (31pp)

S3D: What Opportunities Exist?

mixavg_transport_m.f90

```fortran
diffFlux(:,:,:,n_spec,:) = 0.0
DIRECTION: do m=1,3
  SPECIES: do n=1,n_spec-1

    if (baro_switch) then
      ! driving force includes gradient in mole fraction and baro-diffusion:
      diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * ( grad_Ys(:,:,:,n,m)  &
                          + Ys(:,:,:,n) * ( grad_mixMW(:,:,:,m)    &
                          + (1 - molwt(n)*avmolwt) * grad_P(:,:,:,m)/Press))
    else
      ! driving force is just the gradient in mole fraction:
      diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * ( grad_Ys(:,:,:,n,m)  &
                          + Ys(:,:,:,n) * grad_mixMW(:,:,:,m) )
    endif

    ! Add thermal diffusion:
    if (thermDiff_switch) then
      diffFlux(:,:,:,n,m) = diffFlux(:,:,:,n,m)    &
          - Ds_mixavg(:,:,:,n) * Rs_therm_diff(:,:,:,n) * molwt(n) &
          * avmolwt * grad_T(:,:,:,m) / Temp
    endif

    ! compute contribution to nth species diffusive flux
    ! this will ensure that the sum of the diffusive fluxes is zero.
    diffFlux(:,:,:,n_spec,m) = diffFlux(:,:,:,n_spec,m) - diffFlux(:,:,:,n,m)

  enddo SPECIES
enddo DIRECTION
```

initialize

update

reuse

reuse

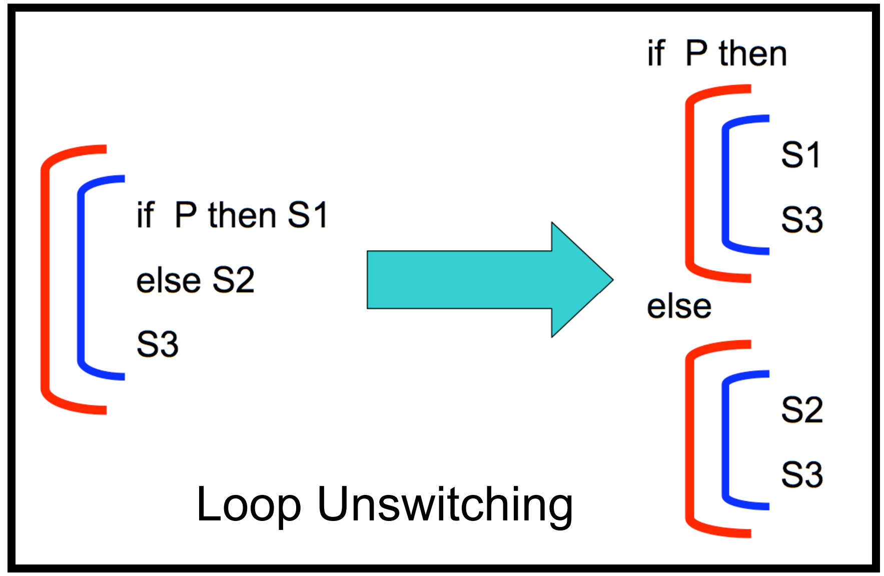
reuse

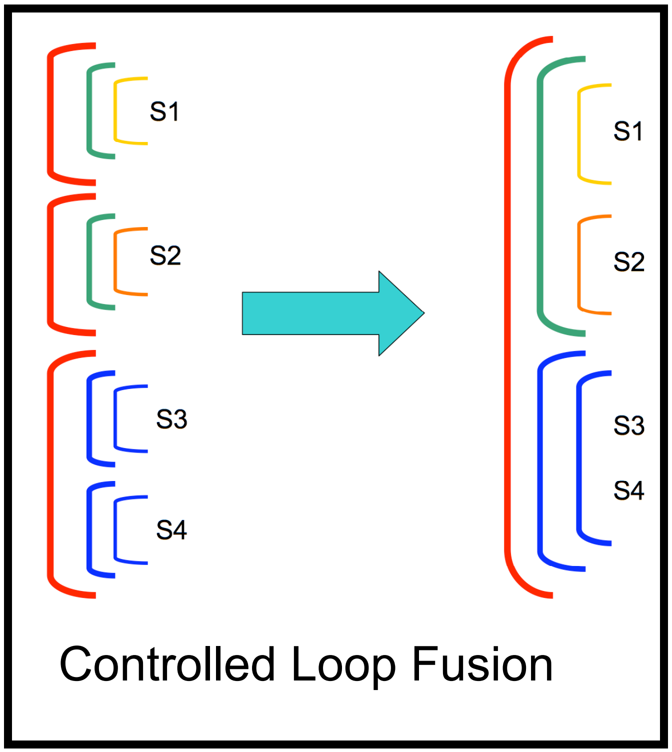
5D loop nest:
2D explicit loops
3D F90 vector syntax

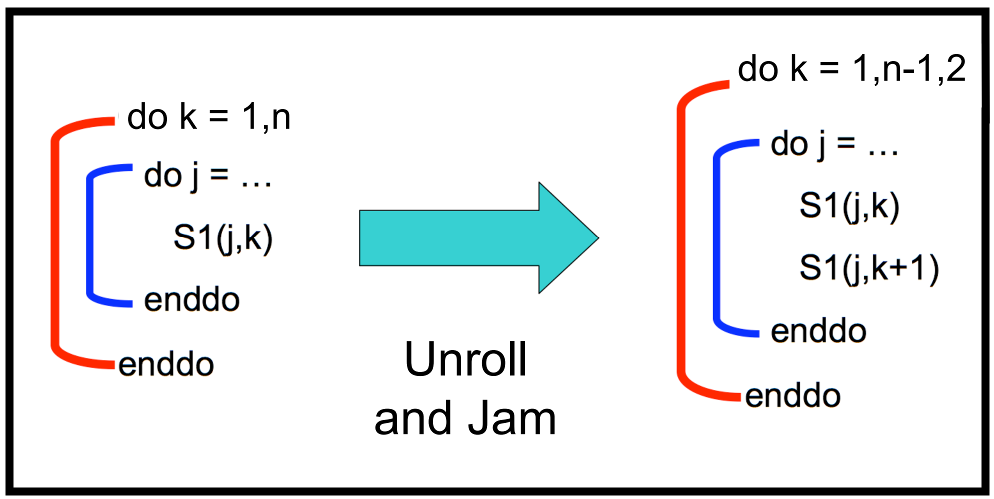
<u>performance problem</u>
data streams
in/out of memory

LoopTool: Loop Optimization of Fortran

Rice University's tool for source-to-source transformation of Fortran
(transformation subset shown)

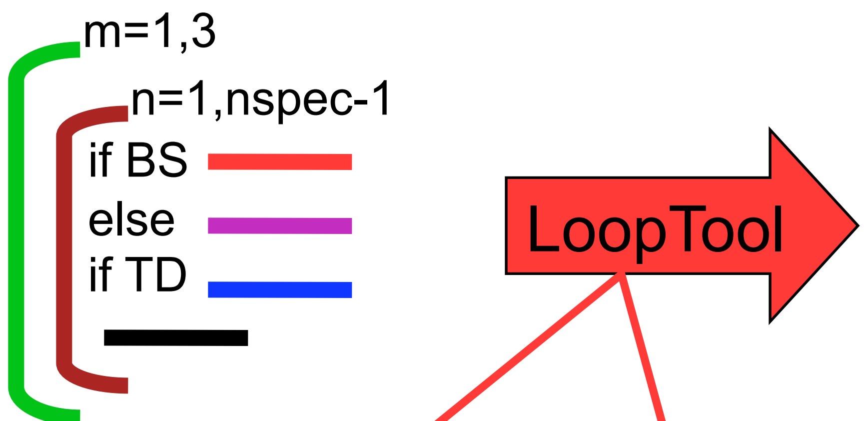




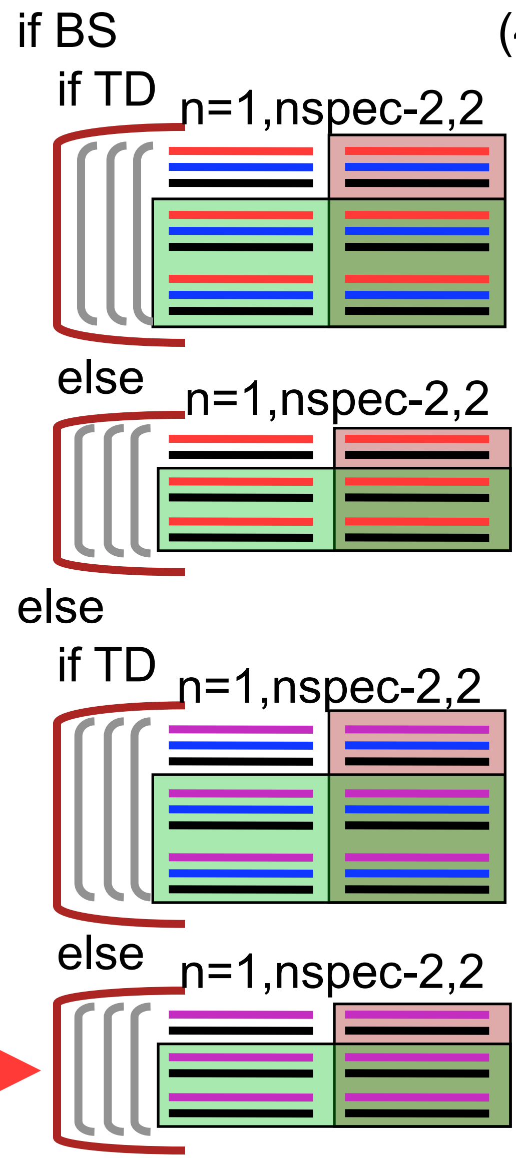


Optimization of S3D Diffusive Flux Loop

(35 lines)



(445 lines)



Transformation Log:

- scalarization (4 stmts)
- loop unswitching (2 conditions)
- fusion (loops within 4 outer nests)
- unroll-and-jam (2 loops)
- peeling excess iterations (4 nests)

2.94x faster than original
(6.7% total savings)

Ongoing Work

- Beginning to study new applications
  - PFLOTRAN, POP
- Modeling toolkit
  - replacing EEL (licensed) with Dyninst toolkit (open source)
    - create open source multi-platform tool
  - status: testing instrumentation using GTC on Opteron platform
- LoopTool
  - being prepared for deployment in 2009