PARSEC and EMGeo

TCG Micro
SSG DPD
NERSC Threading Workshop, March 2015
PARSEC: except for Dev2
PARSEC is a package designed to perform electronic structure calculations of solids and molecules using density functional theory (DFT). The acronym stands for Pseudopotential Algorithm for Real-Space Electronic Calculations. It solves the Kohn–Sham equations in real space, without the use of explicit basis sets.
About PARSEC

- Developed by James Chelikowsky (now at Univ. Texas), Yousef Saad and collaborators at the Univ. Minnesota.

- The distribution available to NERSC scientists and Intel Engineers is not the state-of-the-art PARSEC\textsuperscript{MP} used for cutting-edge simulations by Jim's coworkers.

- Feature and productivity gap exists with PARSEC and PARSEC\textsuperscript{MP}
  - Very common with research codes: scientists' primary goal is \textit{advancing science} not high-performance computing.
  - Constant flux of the developers: graduate students and post docs move on.

- For this workshop, we are going to use PARSEC to
  - Understand the performance issues
  - Discover parallelisms in this class of applications
  - Discuss options for basic to advanced transformation
Recall the processes

- Know your application & define goals
  - Transform PARSEC to attain *sustained performance* with any combination of MPI tasks and OpenMP threads

- Select the target workload and devise experiments
- Incremental development
- Transformative development
- Iterative development while having frequent conversations with Dev2
PARSEC benchmark: 120-atom Carbon Nanotube

```
parsec.in

Boundary_Conditions wire
Boundary_Sphere_Radius 10 ang
begin Cell_shape
  4.2608449866194382 0.0 0.0
end cell_shape
lattice_vector_scale 1 ang
Grid_Spacing: 0.55
States_Num: 728
eigensolver chebdav
corordinate_unit Cartesian_Ang
Correlation_Type ca
Ignore_Symmetry true
Max_Iter 10
Atom_Types_Num: 1
Position of 120 atoms follow
```

ES-2697 2.60 GHz (dual 14-core)
Compilers and libraries
  composer_xe_2015.1.133
  Intel MPI 5.0.2.044
  Use MKL and MKL/FFTW

Performance analysis with MPI
  • Reduced Max_Iter from 100 to 10
  • States_Num from 720 to 728
  • Vary the number of MPI tasks
  • Vary key MPI environments
Scaling investigation on E5-2697 2.60 GHz (dual 14-core)

Compiler options

-march=core-avx2 -O3 -g -ip -qopt-matmul -align array32byte \n-profile-loops=outer -profile-loops-report=2

Runtime options

export OMP_NUM_THREADS=1
export MKL_NUM_THREADS=1
export I_MPI_STATS=ipm
export I_MPI_PIN_DOMAIN=core
export I_MPI_DEBUG=6
#TARBA: topology aware Reduce+Bcast
export I_MPI_ADJUST_ALLREDUCE=4

Elapsed time of 10 iterations

-sec- 800

1 7 14 28

4.2x 3.8x 6.4x

Dgemv Subspace Laplacian
Chebdav_diag Rest

MPI
On the methods used in this scaling study

- **I_MPI_PIN_DOMAIN=core**
  - All the tests are done on a node but our goal is to scale out to multiple nodes using all the resources available. This will set the lower bound of the performance.
  - Domain should be chosen to maximize use of your resources
    - Memory requirements may force to use only a fraction of the cores on a node
    - Resource contentions may override any gain in parallelisms

- **I_MPI_ADJUST_ALLREDUCE and other collectives**
  - Depending upon the message types, the number of tasks and the topology, choosing the right algorithm can be very critical for the performance
  - For this study, 4=topology aware reduce+bcast
  - Subject to OpenMP parallelization algorithms and affinity.
MPI pinning: Core vs Auto

- Auto improves the performance
- Reduced memory contention
- Distributed communication paths

I_MPI_PIN_DOMAIN
• 7C & 14 C: core
• 7A & 14 A: auto
Properties of the Hotspots

- **Dgemv & Laplacian**: limited by memory BW
- **Chebdav_diag**: pure parallel routine
- **subspace & Rest**: mixed bags

Exclusive time (sec)
Respectable MPI scaling but can/must be improved.

 Scaling of 1-7-14 reflects the cost of shared resource: memory bandwidth

 Significant time in MPI with increasing MPI tasks: allreduce

 Why so much time in IFORT (memory allocation) and proportional to MPI tasks?
Bottom-up OpenMP parallelization within a MPI task

- Perform the systematic scaling and performance studies and collect data with tools
- Identify candidate functions and loops for OpenMP parallelization
- Incrementally and iteratively improve the parallel efficiency
- And, make the code easy to understand and maintain for the current and future developers

- Reference MPI calculations with 4 MPI tasks
  - I_MPI_PIN_DOMAIN=auto:7 on E5-2697 (dual socket)
  - I_MPI_PIN_DOMAIN=socket on EX (quad socket)
Easy Targets: Fat Loops

- Loops with large trip counts and computation heavy
  - Do not rely on the loop counts of a serial run
  - Use i) loop counts, ii) call counts and iii) self time vs # of MPI tasks
- Start with the loops with constant counts or $L/N_{\text{MPI}} >> 1$
  - $N_{\text{MPI}}$ is not the number of cores but the target MPI tasks
    - Optimize memory use per task and communication overhead
  - Remove branching and MPI use
  - Rewrite the loops to reduce MPI calls and any serial bottleneck
  - Potential nested OpenMP regions after high-level transformation
  - If blocking can be done, add the outer loops to call each block
## Vtune Bottom-up Function/Call Stack

### MPI=1

<table>
<thead>
<tr>
<th>Function</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>dgemv</td>
<td>271.683s</td>
</tr>
<tr>
<td>orth_normal ← chebdav_diag</td>
<td>146.582s</td>
</tr>
<tr>
<td>dgks ← subspace ← eigval</td>
<td>125.100s</td>
</tr>
<tr>
<td>laplacianmv5</td>
<td>143.688s</td>
</tr>
<tr>
<td>matvec_ke ← matvec1</td>
<td>143.688s</td>
</tr>
<tr>
<td>subspace</td>
<td>103.220s</td>
</tr>
<tr>
<td>eigval ← parsec ← main ← _intel_sssse3_rep_memcpy</td>
<td>103.220s</td>
</tr>
<tr>
<td>chebdav_diag</td>
<td>76.800s</td>
</tr>
<tr>
<td>eigval ← parsec ← main ← _intel_sssse3_rep_memcpy</td>
<td>76.800s</td>
</tr>
<tr>
<td>_intel_memset</td>
<td>16.725s</td>
</tr>
<tr>
<td>expint</td>
<td>11.230s</td>
</tr>
<tr>
<td>_intel_memset</td>
<td>9.114s</td>
</tr>
<tr>
<td>matvec_nloc</td>
<td>6.990s</td>
</tr>
<tr>
<td>laplacianmv1</td>
<td>5.880s</td>
</tr>
<tr>
<td>cheby_filter</td>
<td>4.300s</td>
</tr>
<tr>
<td>dcopy</td>
<td>3.470s</td>
</tr>
<tr>
<td>diagonalmv5</td>
<td>3.360s</td>
</tr>
<tr>
<td>chebdav_diag_IP_cheby_filter2</td>
<td>3.280s</td>
</tr>
<tr>
<td>forclc_wire</td>
<td>2.690s</td>
</tr>
<tr>
<td>lapmvs</td>
<td>2.690s</td>
</tr>
</tbody>
</table>

### MPI=28

<table>
<thead>
<tr>
<th>Function</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>orth_normal ← chebdav_diag ← eigval</td>
<td>13.652s</td>
</tr>
<tr>
<td>dgks ← subspace ← eigval ← parsec</td>
<td>10.160s</td>
</tr>
<tr>
<td>_intel_memset</td>
<td>19.732s</td>
</tr>
<tr>
<td>expint</td>
<td>11.240s</td>
</tr>
<tr>
<td>laplacianmv5</td>
<td>6.691s</td>
</tr>
<tr>
<td>matvec_ke ← matvec1</td>
<td>6.691s</td>
</tr>
<tr>
<td>chebdav_diag_IP_cheby_filter2</td>
<td>3.706s</td>
</tr>
<tr>
<td>cheby_filter ← subspace</td>
<td>2.776s</td>
</tr>
<tr>
<td>eigval ← parsec ← main ← _intel_sssse3_rep_memcpy</td>
<td>2.376s</td>
</tr>
<tr>
<td>cheby_filter ← subspace ← eigval ← parsec</td>
<td>0.399s</td>
</tr>
<tr>
<td>chebdav_diag</td>
<td>0.140s</td>
</tr>
<tr>
<td>cheby_filter1 ← chebdav_diag</td>
<td>0.070s</td>
</tr>
<tr>
<td>subspace</td>
<td>6.441s</td>
</tr>
<tr>
<td>eigval ← parsec ← main ← _libc_s</td>
<td>6.441s</td>
</tr>
<tr>
<td>_I_MPI__intel_sssse3_rep_memcpy</td>
<td>5.361s</td>
</tr>
<tr>
<td>PMPI_Isend</td>
<td>4.599s</td>
</tr>
<tr>
<td>PMPI_Barrier</td>
<td>0.180s</td>
</tr>
<tr>
<td>matvec_nloc</td>
<td>4.457s</td>
</tr>
<tr>
<td>PMPI_Allreduce</td>
<td>0.240s</td>
</tr>
<tr>
<td>chebdav_diag</td>
<td>2.747s</td>
</tr>
<tr>
<td>bdxc_as</td>
<td>2.419s</td>
</tr>
</tbody>
</table>
Loop profile $\text{MPI}=1$

vtune option: 
- knob collection-detail=stack-call-and-tripcount

<table>
<thead>
<tr>
<th>Function</th>
<th>Function file:line</th>
<th>T...</th>
<th>% Time</th>
<th>S...</th>
<th>% Self time</th>
<th>Call count</th>
<th>% Time in loops</th>
</tr>
</thead>
<tbody>
<tr>
<td>orth_normal</td>
<td>tmp/mpifort-ffff-15.0.1.mporth_normal.tmp.f90:20</td>
<td>38...</td>
<td>21.46</td>
<td>38...</td>
<td>21.46</td>
<td>427</td>
<td>21.46</td>
</tr>
<tr>
<td>matvec_interface_mp_laplacianmv5_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/matvec.tmp.f90:1675</td>
<td>35...</td>
<td>20.17</td>
<td>35...</td>
<td>20.17</td>
<td>17,906</td>
<td>20.17</td>
</tr>
<tr>
<td>dgks_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/dgks.tmp.f90:17</td>
<td>32...</td>
<td>18.29</td>
<td>32...</td>
<td>18.29</td>
<td>4</td>
<td>18.29</td>
</tr>
<tr>
<td>subspace_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/subspace.tmp.f90:16</td>
<td>84...</td>
<td>47.56</td>
<td>29...</td>
<td>16.39</td>
<td>4</td>
<td>16.39</td>
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<tr>
<td>chebdav_diag</td>
<td>tmp/mpifort-ffff-15.0.1.mp/chebdav.tmp.f90:26</td>
<td>85...</td>
<td>47.89</td>
<td>23...</td>
<td>13.03</td>
<td>1</td>
<td>13.03</td>
</tr>
<tr>
<td>matvec_interface_mp_matvec_ke_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/matvec.tmp.f90:702</td>
<td>41...</td>
<td>23.23</td>
<td>47...</td>
<td>2.69</td>
<td>20,904</td>
<td>2.19</td>
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<tr>
<td>matvec_interface_mp_matvec_nloc_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/matvec.tmp.f90:204</td>
<td>31...</td>
<td>1.76</td>
<td>31...</td>
<td>1.76</td>
<td>20,904</td>
<td>1.41</td>
</tr>
<tr>
<td>forceion_wire</td>
<td>forceion_wire.f90:12</td>
<td>30...</td>
<td>1.73</td>
<td>30...</td>
<td>1.73</td>
<td>1</td>
<td>1.73</td>
</tr>
<tr>
<td>chebdav_diag_IP_cheby_filter2_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/chebdav.tmp.f90:1233</td>
<td>21...</td>
<td>12.27</td>
<td>19...</td>
<td>1.10</td>
<td>426</td>
<td>1.10</td>
</tr>
<tr>
<td>eigval_</td>
<td>eigval.f90:15</td>
<td>1...</td>
<td>95.47</td>
<td>3...</td>
<td>0.00</td>
<td>5</td>
<td>0.00</td>
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<tr>
<td>matvec_interface_mp_matvec1_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/matvec.tmp.f90:37</td>
<td>44...</td>
<td>24.99</td>
<td>16...</td>
<td>0.00</td>
<td>20,904</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Function</th>
<th>Function file:line</th>
<th>...</th>
<th>% Time</th>
<th>...</th>
<th>% Self</th>
<th>Loop ent...</th>
<th>Min ite...</th>
<th>Avg iterat...</th>
<th>Max ite...</th>
</tr>
</thead>
<tbody>
<tr>
<td>orth_normal</td>
<td>tmp/mpifort-ffff-15.0.1.mporth_normal.tmp.f90:20</td>
<td>21.50</td>
<td>21.50</td>
<td>427</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>62</td>
<td></td>
</tr>
<tr>
<td>chebdav_diag</td>
<td>tmp/mpifort-ffff-15.0.1.mp/chebdav.tmp.f90:26</td>
<td>46.90</td>
<td>13.00</td>
<td>1</td>
<td>426</td>
<td>426</td>
<td>426</td>
<td>426</td>
<td></td>
</tr>
<tr>
<td>subspace_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/subspace.tmp.f90:16</td>
<td>11.10</td>
<td>9.80</td>
<td>4</td>
<td>728</td>
<td>728</td>
<td>728</td>
<td>66</td>
<td></td>
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<tr>
<td>subspace_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/subspace.tmp.f90:16</td>
<td>5.20</td>
<td>5.20</td>
<td>4</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>forceion_wire</td>
<td>forceion_wire.f90:12</td>
<td>1.70</td>
<td>1.70</td>
<td>1</td>
<td>120</td>
<td>120</td>
<td>120</td>
<td>120</td>
<td></td>
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<tr>
<td>matvec_interface_mp_matvec_nloc_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/matvec.tmp.f90:204</td>
<td>1.30</td>
<td>1.30</td>
<td>20,904</td>
<td>1</td>
<td>4</td>
<td>4</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>matvec_interface_mp_matvec_ke_</td>
<td>tmp/mpifort-ffff-15.0.1.mp/matvec.tmp.f90:702</td>
<td>21.60</td>
<td>1.10</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>12</td>
<td></td>
</tr>
</tbody>
</table>

1853
Planned actions based on the performance data

1. **dgks & ortho_normal**
   - Combined 40% (1) and 20% (28), the prime target
   - Each call is expensive and uses gemv

2. **laplacianmv5: not laplacianmv5 but callers**
   - Constant (max iterations * MPI) : 1853*28=51870
   - Threads not helpful: large call counts, same for any MPI; per call < 10 msec
   - Better to move up to the caller: **matvec_ke**
   - Candidate for SIMD (not going to do anything more for this workshop)

3. **subspace**

4. **chebdav_diag**
Laplacianmv5

- Computing the kinetic energy by Finite-Difference method
- EMGeo: FD & QMR
- Loops over parallel%mydim
- Update q1(irow),...,q5(irow) by reduction
- ish/j inner loops: thread private

Similar to EMGeo

do i=1,n; ...; enddo
subroutine zlaplacianmv5(solver, parallel, neibs, tneibs, chi, coe2, &
p1, p2, p3, p4, p5, q1, q2, q3, q4, q5)

!skip INTENT(IN): solver, parallel, neibs, tneibs, chi, coe2
SCALAR, dimension(parallel%wedge+1): p1, p2, p3, p4, p5
SCALAR, dimension(parallel%ldn): q1, q2, q3, q4, q5
!Local variables
SCALAR :: coef, chi1, chi2, tmp1, tmp2, tmp3, tmp4, tmp5
INTEGER idx1, idx2, i, j, jj, ish, irow, term1, term2, mydim
mydim = parallel%mydim !Local copy
if (parallel%lap_dir_num == 0) then
  term1 = 6
  if (even == 0) then
    if (solver%nrep == 1) then
      do i = 1, mydim
        1row = parallel%pint(i)
        do ish = 1, solver%norder, 2
          do j = 1, 3
            enddo
        enddo
        q1(irow) = q1(irow) + tmp1
        .......
        q5(irow) = q5(irow) + tmp5
      enddo
    else
      !!!similar loop
    endif
    if (solver%nrep == 1) then
      !!!similar loop
    else
      !!!similar loop
    endif
    !!!similar loop
  endif
else
  term1 = 6+2*parallel%lap_dir_num
  if (solver%nrep == 1) then
    !!!similar loop
  else
    !!!similar loop
  endif
end subroutine zlaplacianmv5
But wait, we know everything about PARSEC: algorithms, data distributions, parallelisms ....

- It is just another electronic structure code solving the Kohn-Sham equation!
  - Many good practices and parallel approaches are applicable.
- But, PARSEC is distinct from other ES codes:
  - A finite-difference method on a 3D regular mesh for the kinetic energies.
  - Chebyshev-filtered subspace iteration method during SCF cycles.

Time for really serious discussions with Dev2 and future-proof PARSEC

- What are the performance goals?
- Can the proposed code modifications be broadly applied by all the contributing developers, now and future and work on most of the systems where PARSEC will be used?
- Is anything else to consider before committing to the changes?
EMGeo: Advanced
Recap of EMGeo

- Employs QMR on a complex vector \( \hat{y} = A \hat{x} \)
- Loops followed by Allreduce -> OMP PARALLEL DO
- ELLPACK-format of \( A \)
  - \( ncol(i) < ncol_{\text{max}} \) : # of non-zero columns per row
  - \( ncol_{\text{max}} \) set by the dimension (3D), the order of stencil operator, real/complex
  - Invalid columns (zeros) are masked; good for vector machine*
- Blas I operations with Krylov subspace vectors
  - Ensuring alignment of all the vectors and SIMD clause will be sufficient for the performance.

* Iterative methods for sparse linear systems, Yousef Saad, p86. 1996, PWS publishing
Data Partition: maximize locality

EMGeo employs a spatial decomposition of a 3D cell by \( I*J*K \)

- Each cube on a MPI can be further partitioned: \( i*j*k \)
  - Hard to find \((i,j,k)\) for \((l%i==0 \land J%j==0 \land K%k ==0)\).

- Most of the critical loops do not expose the underlying data partition: the local data on a task is serialized.

- Reorder the sparse matrix to maximize data locality and facilitate vectorization
  - Spatially order the rows and block them by SIMD length
  - Z-order curve-filling method to order the spare matrix
  - Widely used: LAMMPS, QCD, ...

Optimizing SpMV

- Allow compiler optimizations

```
!$OMP PARALLEL DO REDUCTION(+:ay),&
!$OMP PRIVATE(csum,mcole,j)
  do i=1,n
    ay = ay + cpnt(i)*dconjg(cpnt(i))
    csum = czero
    mcole=lshift(rshift(mcol(i),1),1)
    do j=1,mcole,2
      csum = csum + mtx(j,i)*cgs(index(j,i))
      csum = csum + mtx(j+1,i)*cgs(index(j+1,i))
    enddo
  if(mcole.ne.mcol(i))
    csum = csum+mtx(mcol(i),i)*cgs(index(mcol(i),i))
    cvkl(i) = csum
  enddo
!$OMP END PARALLEL DO
```

Now

```
!$OMP PARALLEL REDUCTION(+:ay),&
!$OMP PRIVATE(csum,mcole,j,i,ip,ay_t)
  ip=omp_get_thread_num();
  ay_t=0.0d-
  do i=voffset(ip),voffset(ip+1)
    ay_t = ay_t + cpnt(i)*dconjg(cpnt(i))
  enddo
  ay = ay + ay_t
  do i=voffset(ip),voffset(ip+1)
    csum = czero
    !$OMP SIMD REDUCTION(csum)
    do j=1,mcol(i)
      csum = csum + mtx(j,i)*cgs(index(j,i))
    enddo
    cvkl(i) = csum
  enddo
!$OMP END PARALLEL
```

- voffset(ip), the pre-computed starting row for the ip thread
- Control cache blocking and adapt to cache modes
- Reorder index to optimize gather operations

All done at the code design step.
Revisiting ELLPACK format in EMGeo: Dev4

- ELLPACK format has been widely used for vector architectures including GPUs
- Use two auxiliary integer arrays to inquire non-zero elements per row i
  - mcol(1:n), mcol(i) < mcol_max, mcol_max=12
  - index(mcol_max,n)
- The number of unique grid points is n/3: at (x,y,z), 3D EM vector
- How to pack mcol_max*2 doubles for 4,8,16, ... way SIMD?
- BTW, is the double precision really necessary except for the reductions?
Lattice QCD with Domain Decomposition on Intel® Xeon Phi™ Co-Processors

Simon Heybrock*, Bálint Joó†, Dhiraj D. Kalamkar‡, Mikhail Smelyanskiy§, Karthikeyan Vaidyanathan‡, Tilo Wettig*, and Pradeep Dubey§
*Institute for Theoretical Physics, University of Regensburg, Germany
†Thomas Jefferson National Accelerator Facility, Newport News, VA, USA
‡Parallel Computing Lab, Intel Corporation, Bangalore, India
§Parallel Computing Lab, Intel Corporation, Santa Clara, CA, USA

http://dl.acm.org/citation.cfm?id=2683602
https://github.com/JeffersonLab/qphix
Data distribution and cache blocking

- collapse(2) over the outer loops of the triple loop
- Cache blocking
### SIMD-Friendly Data Layout

**Scanline: SOALEN sites along X**

<table>
<thead>
<tr>
<th>24-components</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_0 )</td>
<td>( e_0 \ldots e_{SL-1} \ldots e_{</td>
</tr>
<tr>
<td>( c_1 )</td>
<td>( e_0 \ldots e_{SL-1} \ldots e_{</td>
</tr>
<tr>
<td>( \ldots )</td>
<td>( \ldots \ldots \ldots )</td>
</tr>
<tr>
<td>( c_{23} )</td>
<td>( e_0 \ldots e_{SL-1} \ldots e_{</td>
</tr>
</tbody>
</table>

- Partial SOA: transpose part of each scanline
- Efficient SIMD across sites is possible if \( SL \% VLEN = 0 \)
- Less TLB pressure
- Complicates address calculations for \( x \)-neighbors
Load-balanced Efficient Cache Blocking

- Load balancing: mainly due to non power of 2 cores
- Solution: multi-phase block allocation
  - No. of blocks more than cores => allocate round robin to all cores
  - When no. of blocks less than cores,
    - either split in T: make more blocks than cores
    - just allocate remaining blocks and finish
    - heuristic to terminate process: when T gets small
Disruptive change is coming – and the time to act is right now.
Conclusions

- Time to future-proof your HPC applications!
- Think what made your MPI applications great.
- OpenMP*/MPI for clusters of SMPs
  - Provide fast path to high-performance parallel computing
  - Maximize productivity of the developers and community
  - Optimize use of shared & distributed resources
  - Leverage open standards and expanding ecosystems
- Principles of high-performance parallel programming are keys.
- Software engineering and code design matter.
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