

Accelerated Chemical Kinetics for GEOS-Chem with Kppa

John C. Linford

jlinford@paratools.com

ParaTools, Inc.

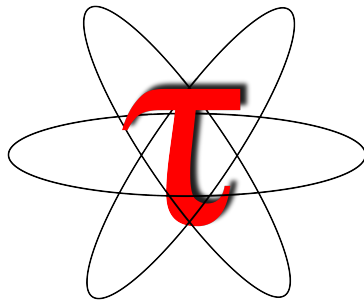
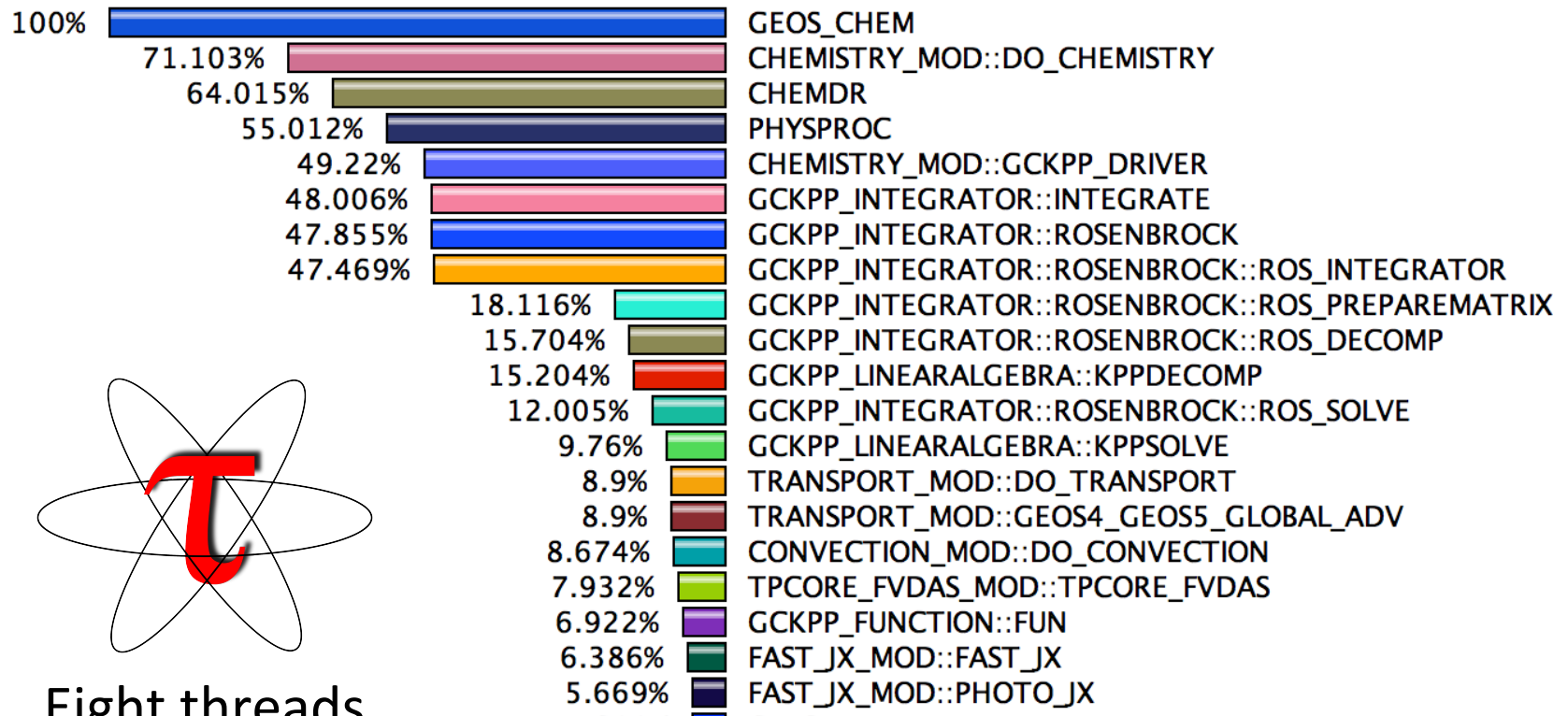
IGC7, Harvard SEAS, Cambridge, MA

4 May 2015

70% of GEOS-Chem Runtime is Chemistry

Metric: TIME

Value: Inclusive percent



Eight threads

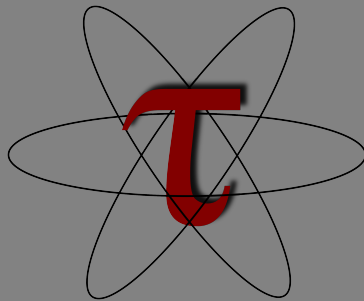
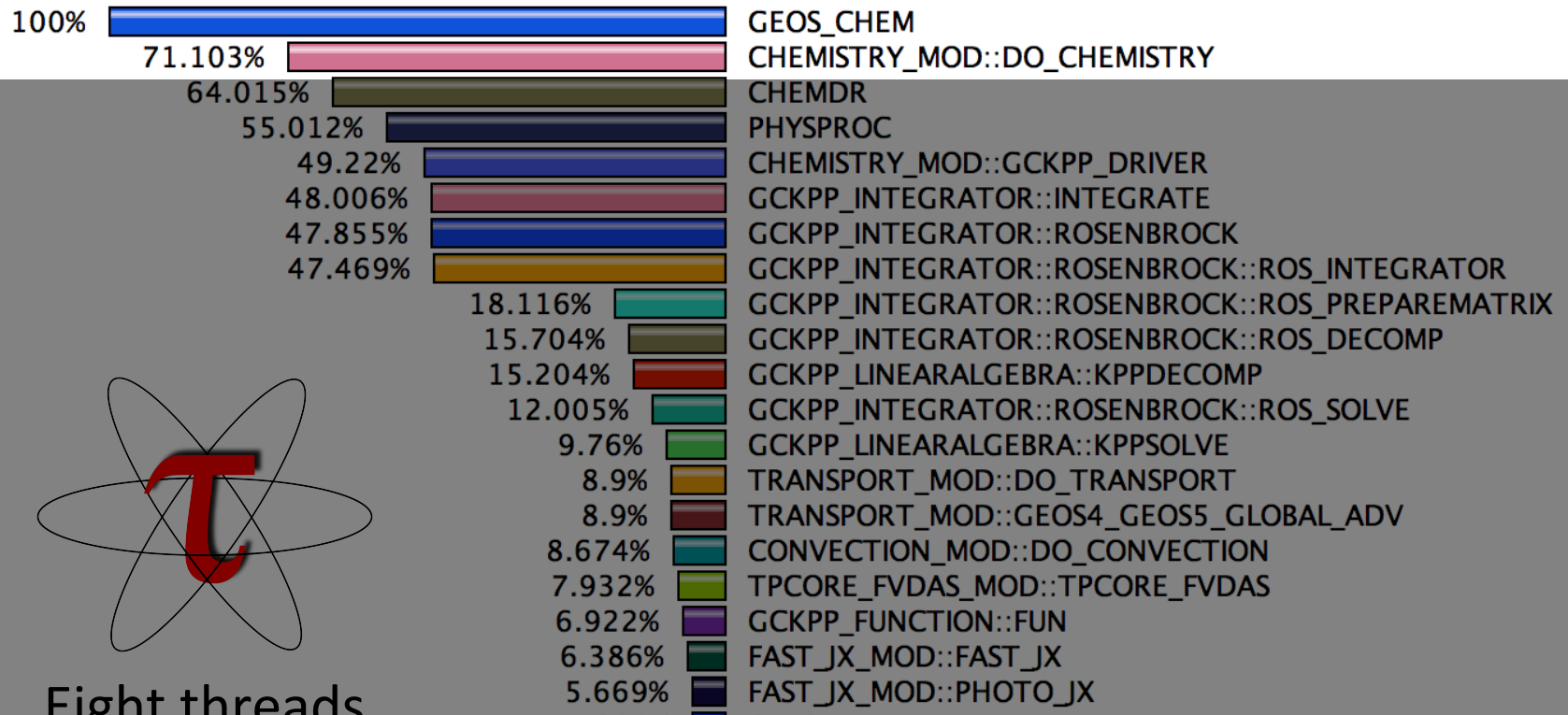
Intel Core i7-4820K CPU

3.70GHz

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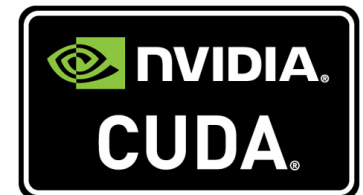
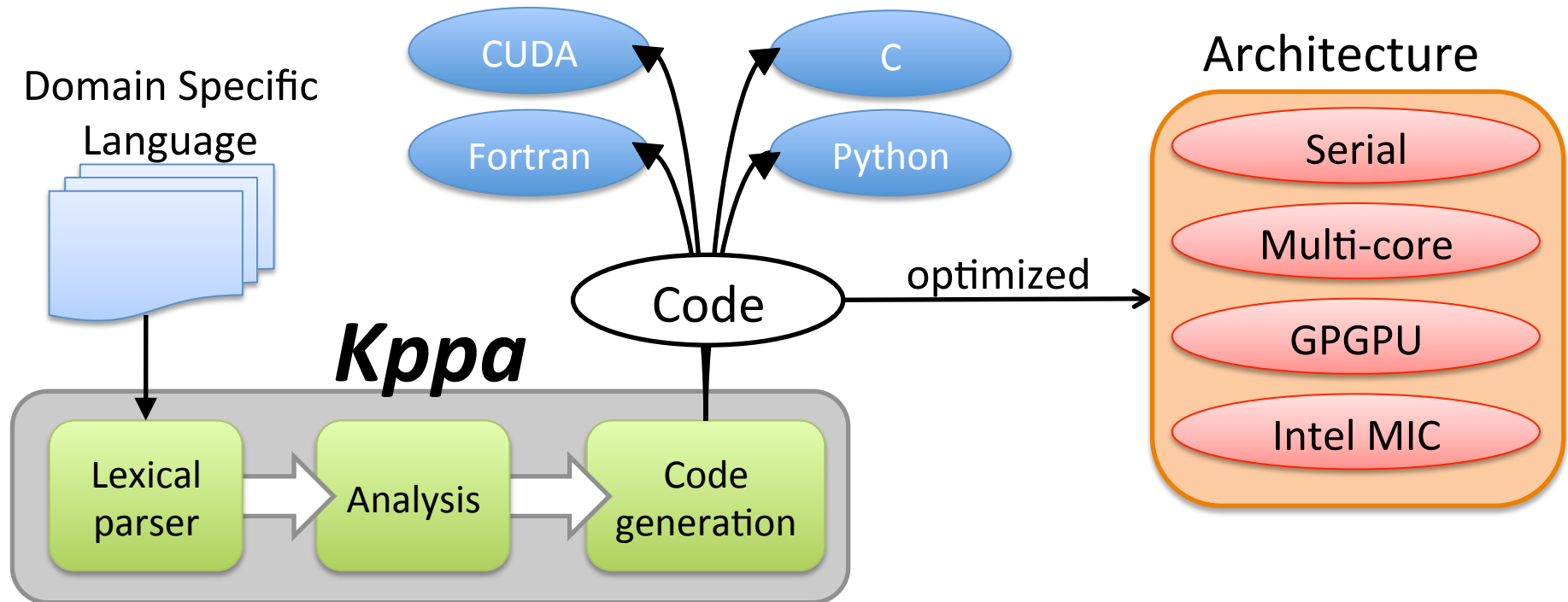


Eight threads

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Kppa: The Kinetic PreProcessor Accelerated



Sparse Matrix/Vector Code Generation

```
<%  
d_Decomp.begin()  
  
piv = lang.Variable('piv', REAL,  
                   'Row element divided by diagonal')  
piv.declare()  
%>  
    ${size_t} idx = blockDim.x*blockIdx.x+threadIdx.x;  
    if(idx < ${ncells32}) {  
        ${A} += idx;  
    }  
    <%  
    lang.upindent()  
    for i in xrange(1, nvar):  
        for j in xrange(crow[i], diag[i]):  
            c = icol[j]  
            d = diag[c]  
            piv.assign(A[j*ncells32] / A[d*ncells32])  
            A[j*ncells32].assign(piv)  
        ...  
    }  
    <% d_Decomp.end() %>
```

Generates C, C++, CUDA,
Fortran, or Python



```
A[334] = t1;  
A[337] = -A[272]*t1 + A[337];  
A[338] = -A[273]*t1 + A[338];  
A[339] = -A[274]*t1 + A[339];  
A[340] = -A[275]*t1 + A[340];  
t2 = A[335]/A[329];  
A[335] = t2;  
A[337] = -A[330]*t2 + A[337];  
A[338] = -A[331]*t2 + A[338];  
A[339] = -A[332]*t2 + A[339];  
A[340] = -A[333]*t2 + A[340];  
t3 = A[341]/A[59];
```

Simplify Before Generating Code

$$\frac{x^3 + x^2 - x - 1}{x^2 + 2x + 1} \equiv x - 1$$

```
x[27] = ((A[43]*A[43]*A[43]) + (A[43]*A[43]) - (A[43]) - (5+4)) /  
        (A[43]*A[43] + (8-6)*A[43] + 1)
```

Simplify

Fortran

```
x(28) = A(44) - 1
```

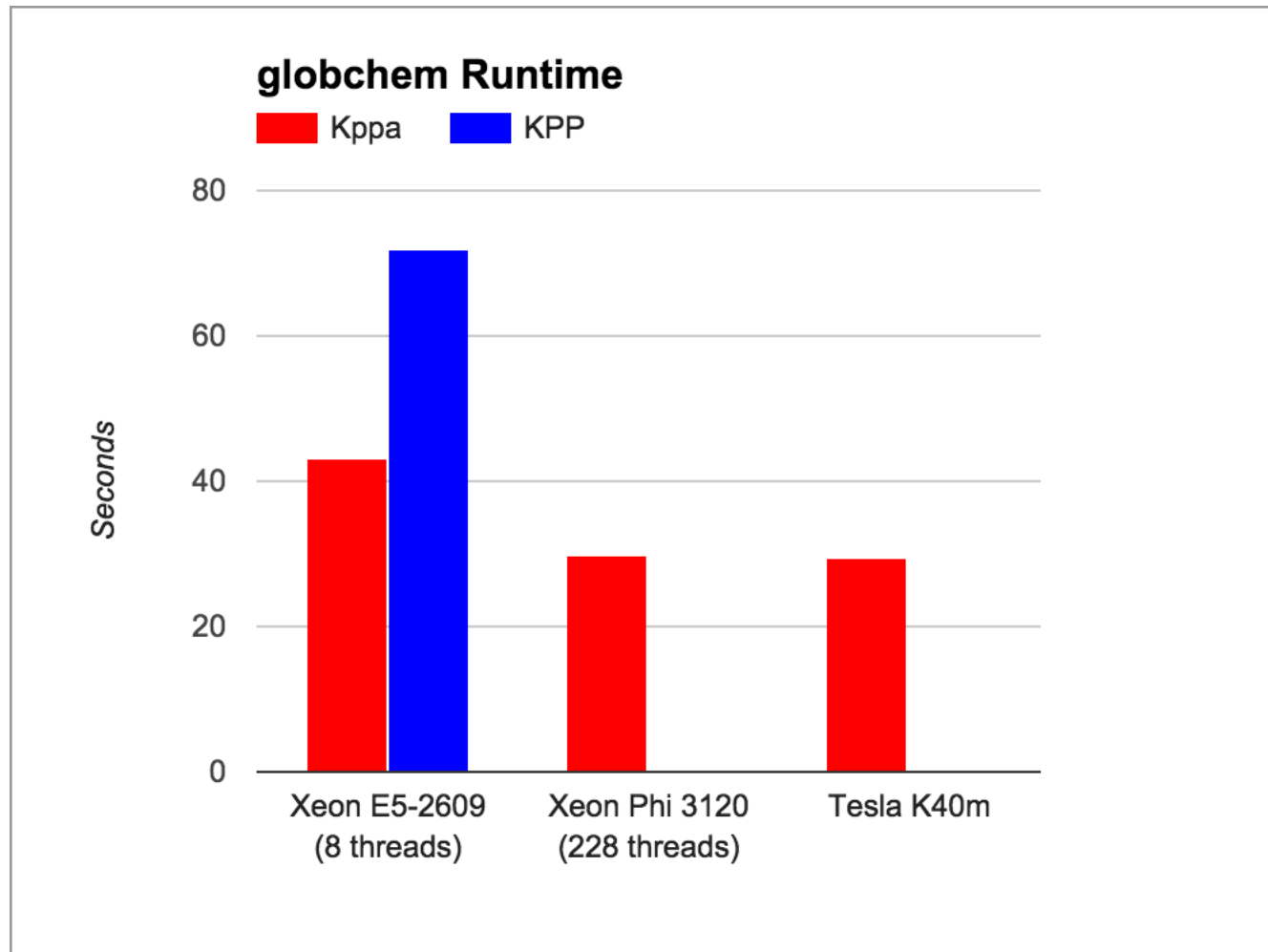
Performance Results

- **Baseline:** hand-tuned KPP-generated code
 1. Use KPP to generate a serial code
 2. A skilled programmer parallelizes the code
- **Comparison:** unmodified Kppa-generated code
 - Same input file format as KPP
 - Little or no modification to source
- **Results:**
 - **Xeon Phi: 140% faster**
 - **NVIDIA K40: 160% faster**
 - **Xeon with OpenMP: 60% faster**

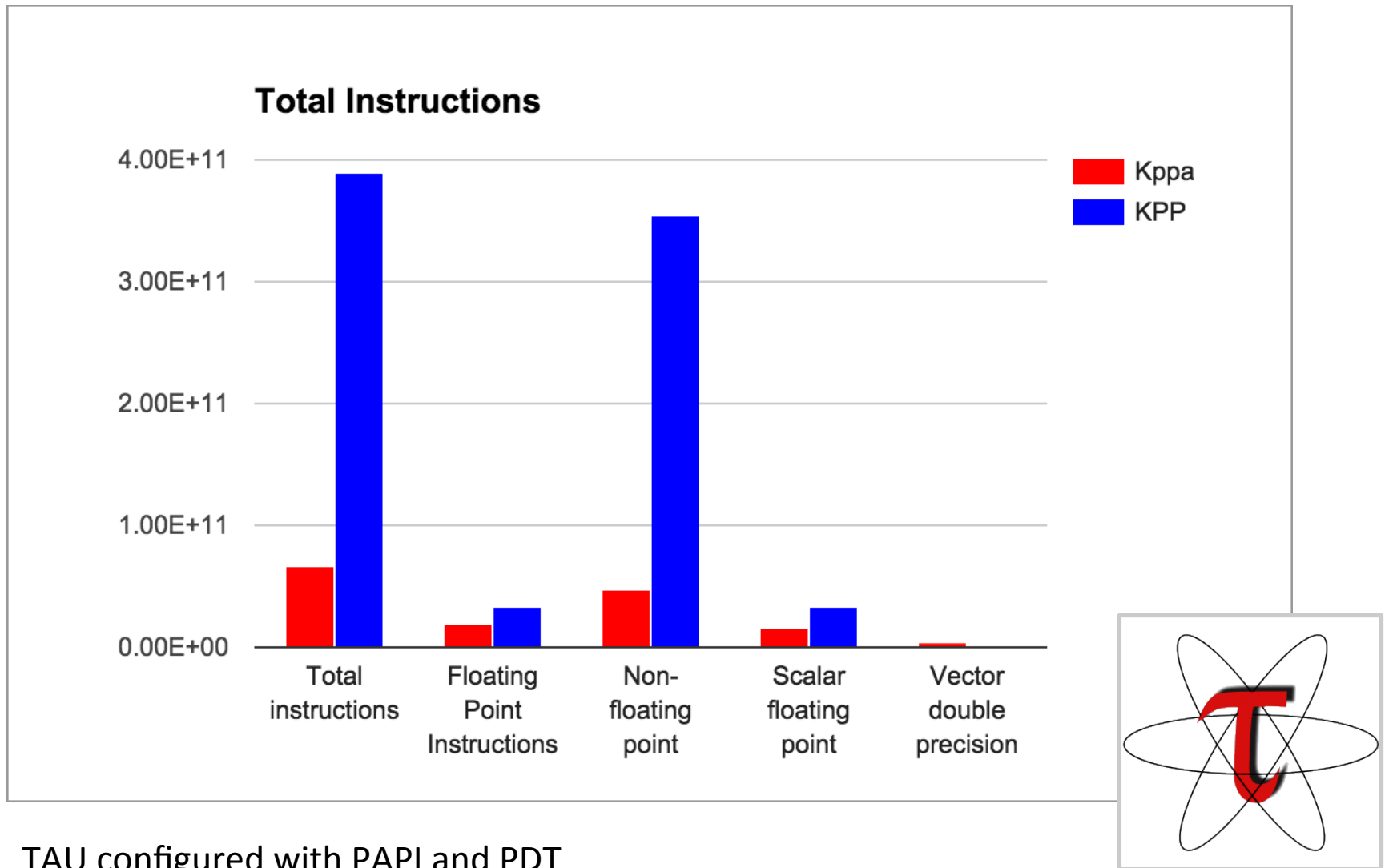


Exact same hardware

Performance Results



Fewer Operations, Faster Runtimes



COSMO-ART Benchmarks

Will Sawyer, *Charles Joseph* (CSCS)

# PEs = 16 (Piz Daint)	2 nodes, 8 MPI tasks/node, nprocx=nproc=4			
	KPP-2.2.3	KPPA-0.2.1 (Serial)	KPPA-0.2.1 (OpenMP, 1 th.)	KPPA-0.2.1 (OpenMP, 2 th.)
Total time (s)	2,198	1,591	1,586	1,311
Integrator time (s)	1,267	1,151	1,144	878
ETS (J)	425,457	357,743	355,058	284,934
Device ETS (J)	62,809	54,027	47,982	36,824
Energy-to-solution (J)	488,265	411,770	403,040	321,758
Integrator function calls	2,649,358,944	2,789,654,372	2,789,654,372	2,789,654,372
Integrator <u>jacobian</u> calls	662,339,736	697,413,593	697,413,593	697,413,593
Integrator steps	662,339,736	697,413,593	697,413,593	697,413,593
Integrator accepted steps	662,339,736	697,413,593	697,413,593	697,413,593
Integrator rejected steps	0	0	0	0
Integrator LU decompositions	662,339,736	697,413,593	697,413,593	697,413,593
Integrator forward/backward substitutions	2,649,358,944	2,789,654,372	2,789,654,372	2,789,654,372
Integrator singular matrix decompositions	0	0	0	0
# PEs = 48 (Piz Dora)	2 nodes, 24 MPI tasks/node, nprocx=8 nproc=6			
	KPP-2.2.3	KPPA-0.2.1 (Serial)	KPPA-0.2.1 (OpenMP, 1 th.)	KPPA-0.2.1 (OpenMP, 2 th.)
Total time (s)	637	449	450	389
Integrator time (s)	331	279	280	217
ETS (J)	223,873	174,409	179,038	142,054
Device ETS (J)	0	0	0	0
Energy-to-solution (J)	223,873	174,409	179,038	142,054
Integrator function calls	2,649,299,600	2,789,645,788	2,789,645,788	2,789,645,788
Integrator <u>jacobian</u> calls	662,324,900	697,411,447	697,411,447	697,411,447
Integrator steps	662,324,900	697,411,447	697,411,447	697,411,447
Integrator accepted steps	662,324,900	697,411,447	697,411,447	697,411,447
Integrator rejected steps	0	0	0	0
Integrator LU decompositions	662,324,900	697,411,447	697,411,447	697,411,447
Integrator forward/backward substitutions	2,649,299,600	2,789,645,788	2,789,645,788	2,789,645,788
Integrator singular matrix decompositions	0	0	0	0

Next Steps

- Partnership with David Topping (Manchester)
 - EMiT 2015 Keynote
 - Horizon 2020 proposal
 - Aerosols
 - MCM
 - Large mechanisms
- Partnership with Will Sawyer (CSCS)
 - PRACE integrator
 - About 4x faster in COSMO-ART

[http://www.paraTools.com/kppa](http://www.paratools.com/kppa)

Downloads, tutorials, resources