

# ParaTools

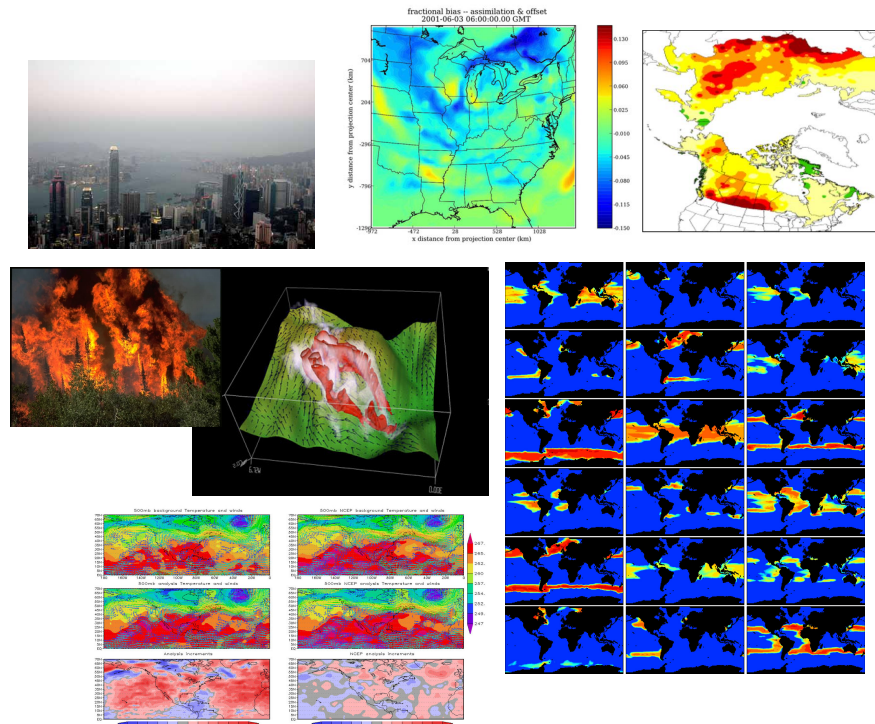


## Kppa The Kinetic PreProcessor Accelerated

November 15, 2012

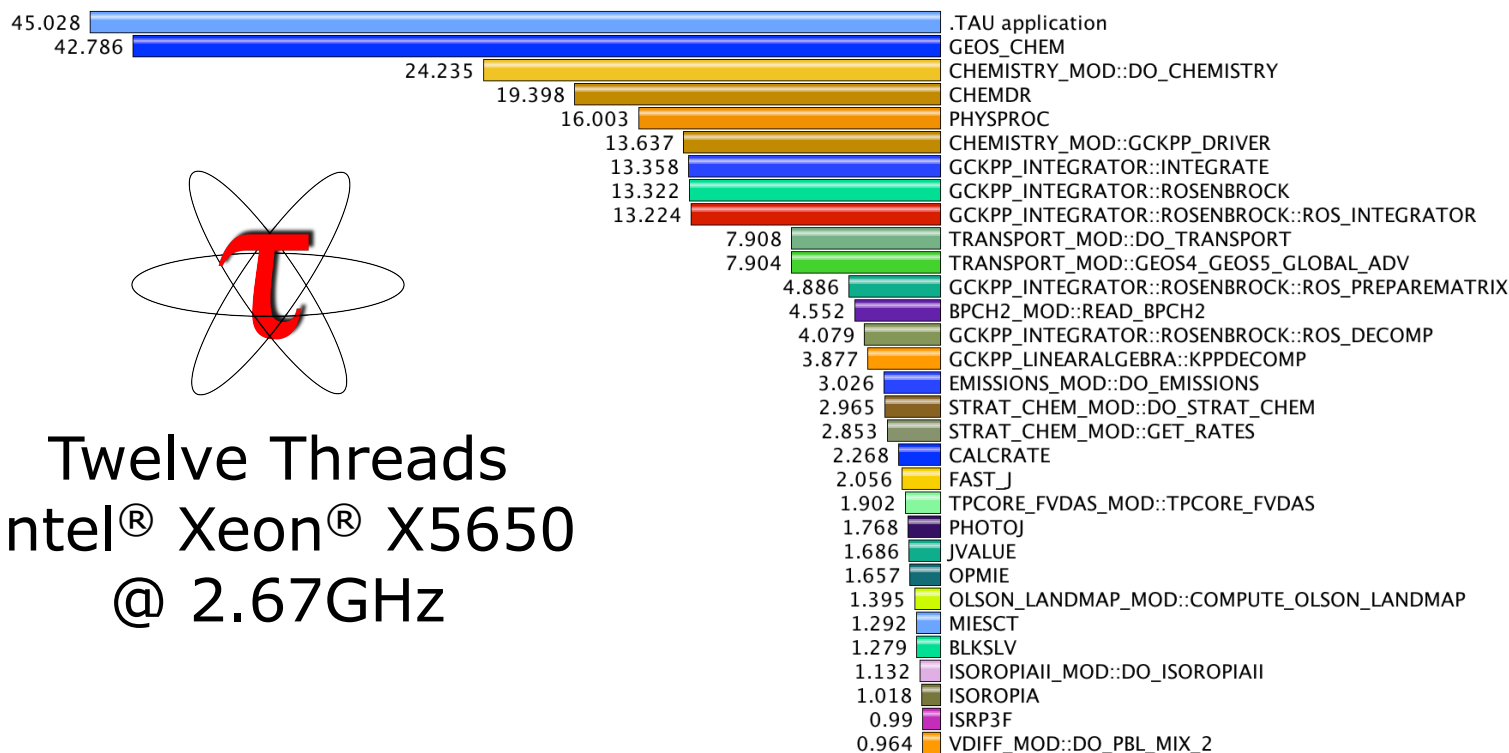
# Chemical Kinetic Simulation

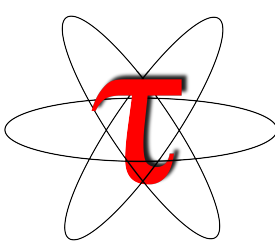
- Pyrolysis and Combustion
- Air and Water Quality
- Climate Change
- Wildfires, Volcanic Eruptions
- Plastics Devolatilzation
- Microorganism Growth
- Cell Biology



# Solving Coupled Stiff ODE Systems is Expensive

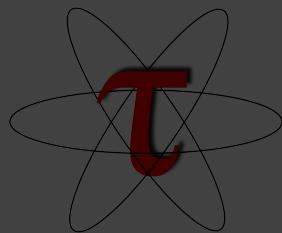
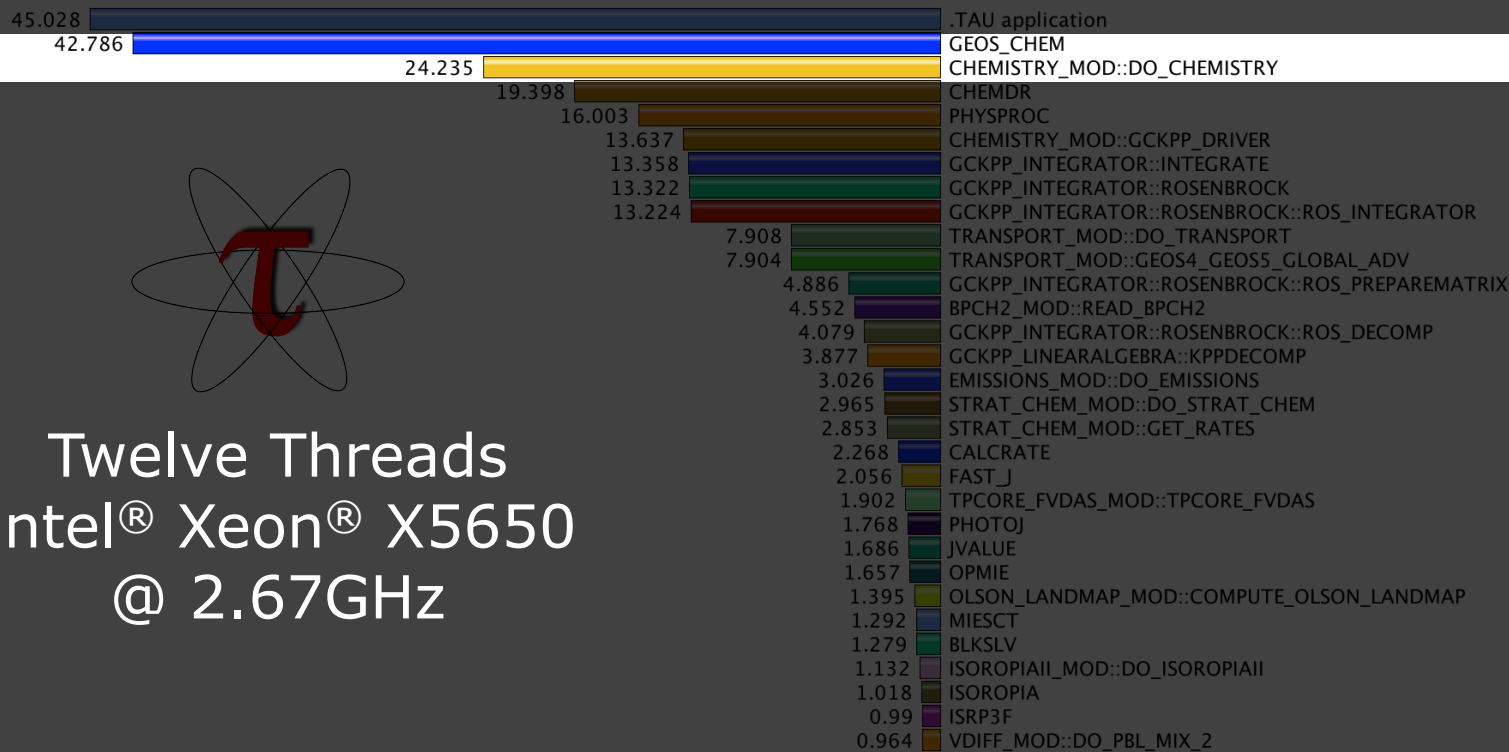
Metric: TIME  
Value: Inclusive  
Units: seconds



  
 Twelve Threads  
 Intel® Xeon® X5650  
 @ 2.67GHz

# Solving Coupled Stiff ODE Systems is Expensive

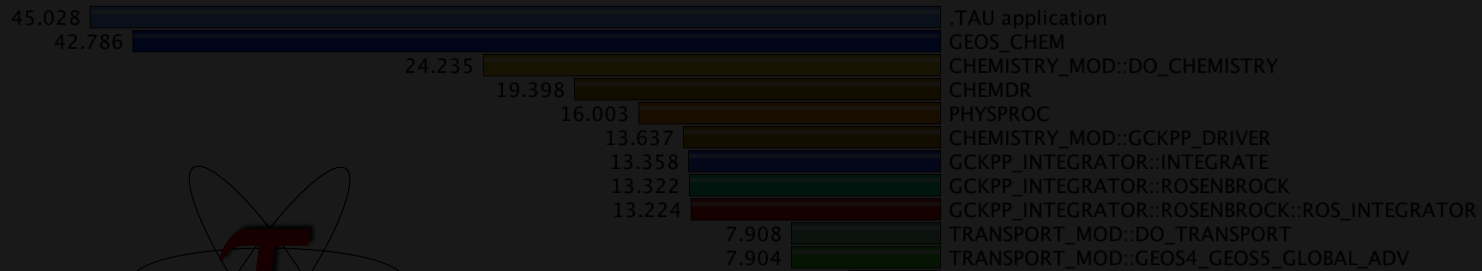
Metric: TIME  
Value: Inclusive  
Units: seconds



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# Solving Coupled Stiff ODE Systems is Expensive

Metric: TIME  
Value: inclusive  
Units: seconds



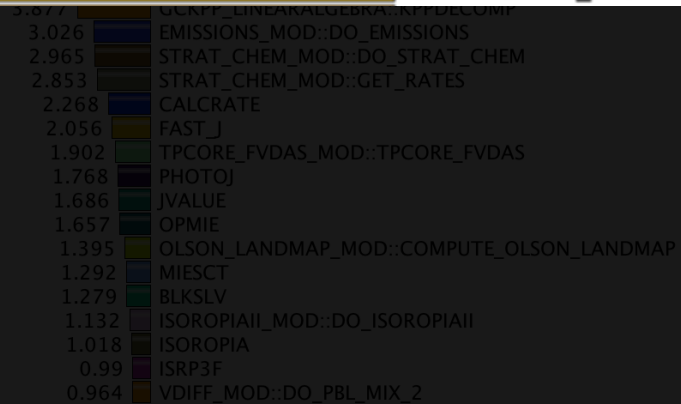
42.786

24.235

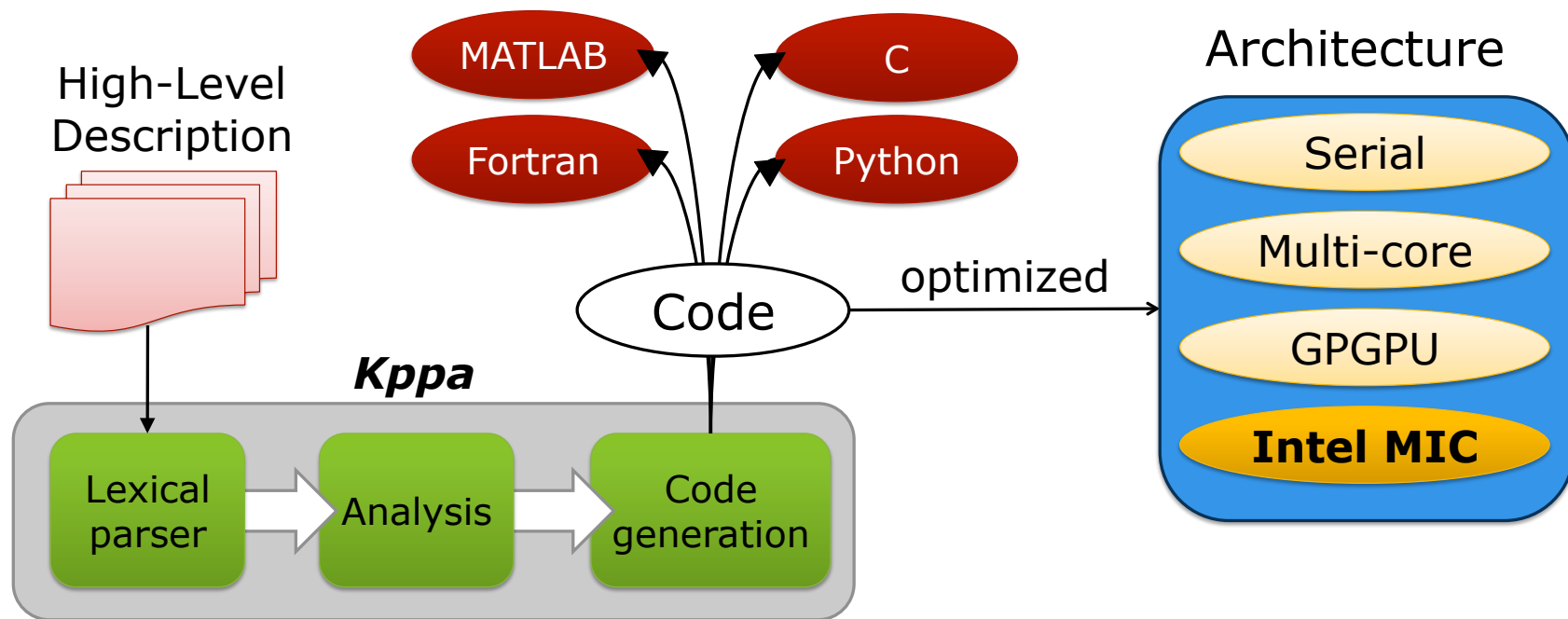
GEOS\_CHEM

CHEMISTRY\_MOD::DO\_CHEMISTRY

Twelve Threads  
Intel® Xeon® X5650  
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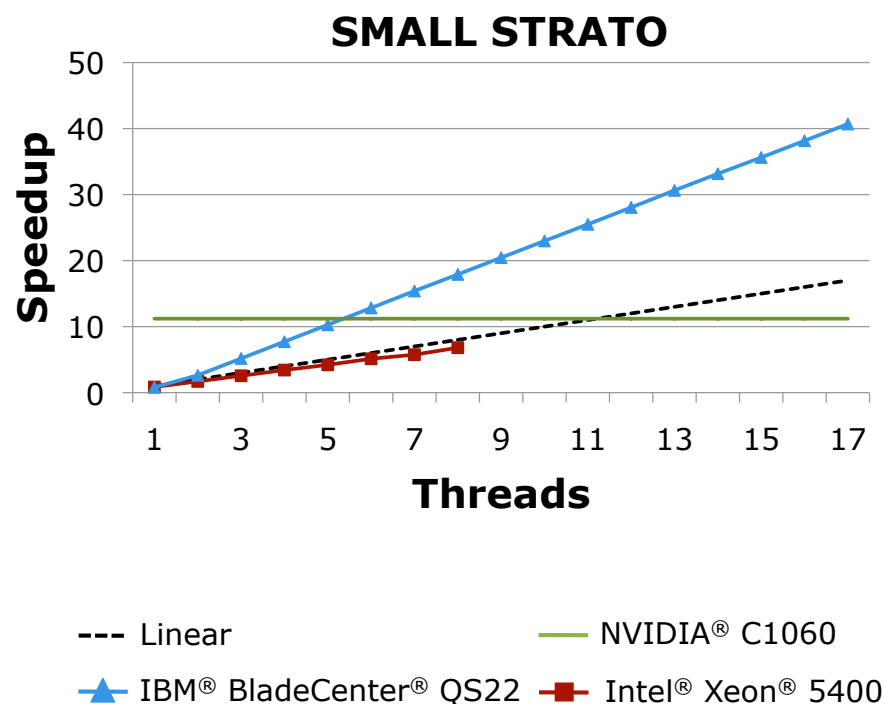


# Kppa: The Kinetic PreProcessor Accelerated



# Kppa-generated can be 40x faster than hand-tuned

- Reorder chemical species to **minimize fill-in**
- Reorder concentration data to **maximize vectorization**
- Reorder grid cells to **reduce excessive iteration**



# Meta-programming for Automatic 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() %>
```



C/C++/CUDA, Fortran

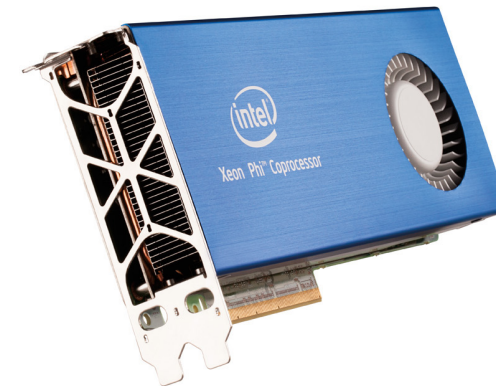
```
A[334] = t1;  
A[337] = -A[272]*t1 + A[337];  
A[338] = -A[273]*t1 + A[338];  
A[339] = -A[274]*t1 + A[339];  
A[340] = -A[275]*t1 + A[340];  
t2 = A[335]/A[329];  
A[335] = t2;  
A[337] = -A[330]*t2 + A[337];  
A[338] = -A[331]*t2 + A[338];  
A[339] = -A[332]*t2 + A[339];  
A[340] = -A[333]*t2 +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



# Kppa's Architecture Parameterization

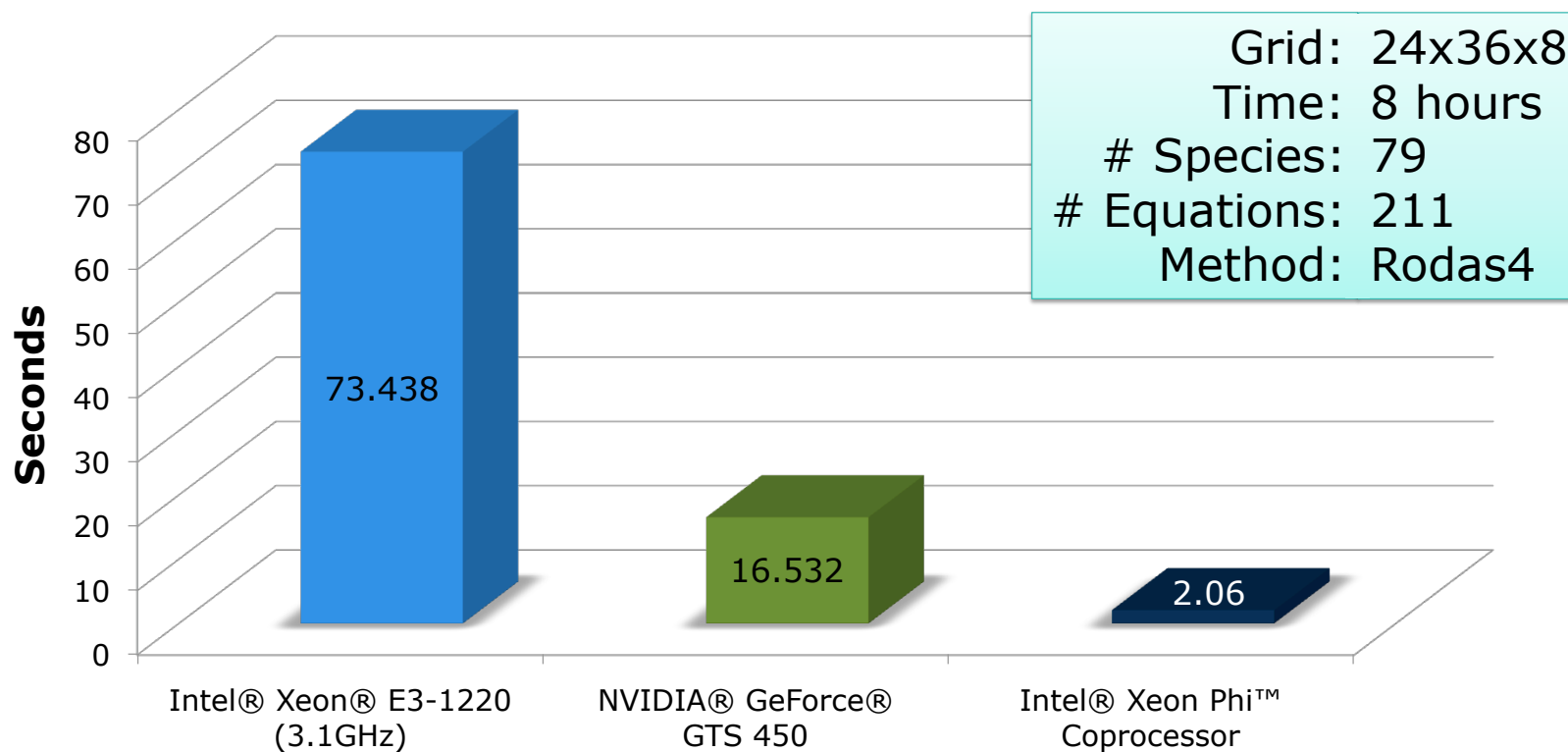
	CPU	GPU	Intel <sup>®</sup> MIC	CBEA
<b>Instruction Cardinality</b>	1	32	16	4
<b>Integrator Cardinality</b>	1	∞	16	4
<b>Scratch Size</b>	N/A	16 KB	N/A	256 KB

Targeting the Intel<sup>®</sup> Xeon<sup>®</sup> Phi<sup>™</sup> coprocessor was easy!



Just had to parameterize the new architecture in Kppa and generate an OpenMP code

## Kppa-generated SAPRC Kernel: 35.6x Speedup



# ParaTools

Download Kppa from  
[www.pاراتools.com/kppa](http://www.paratools.com/kppa)

ParaTools