



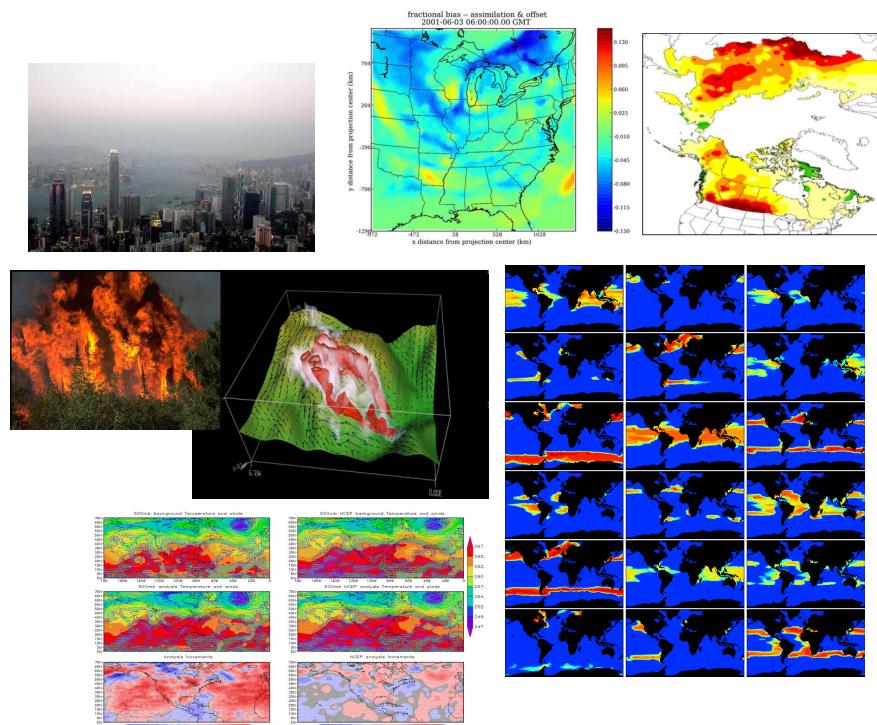
# Kppa

## The Kinetic PreProcessor Accelerated

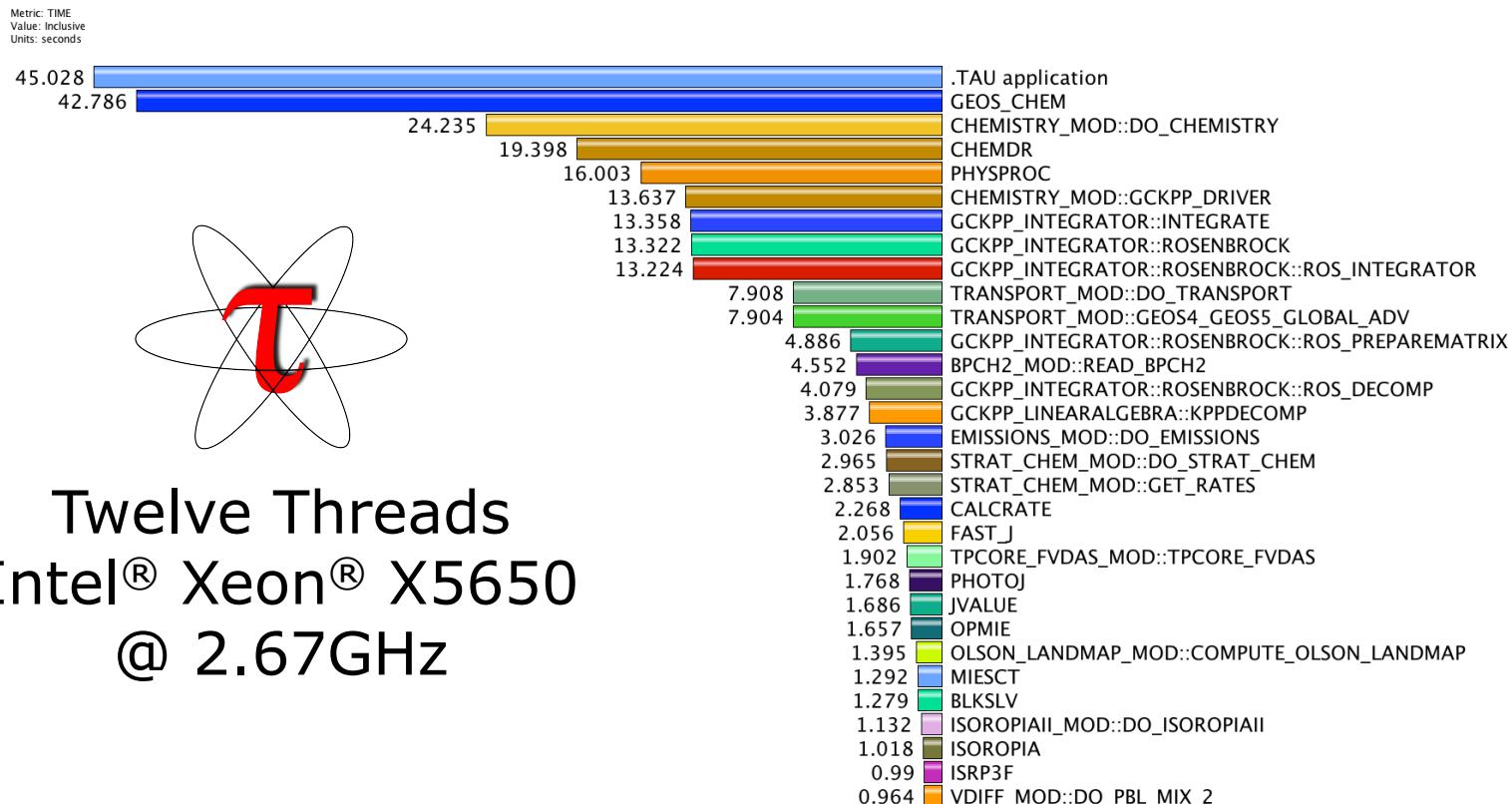
November 15, 2012

# Chemical Kinetic Simulation

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



# Solving Coupled Stiff ODE Systems is Expensive



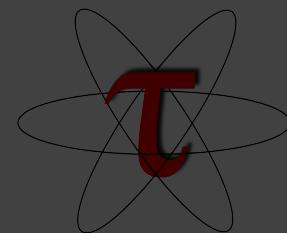
Twelve Threads  
Intel® Xeon® X5650  
@ 2.67GHz

# Solving Coupled Stiff ODE Systems is Expensive

Metric: TIME  
Value: Inclusive  
Units: seconds

45.028  
42.786  
24.235  
19.398  
16.003  
13.637  
13.358  
13.322  
13.224  
7.908  
7.904  
4.886  
4.552  
4.079  
3.877  
3.026  
2.965  
2.853  
2.268  
2.056  
1.902  
1.768  
1.686  
1.657  
1.395  
1.292  
1.279  
1.132  
1.018  
0.99  
0.964

.TAU application  
GEOS\_CHEM  
CHEMISTRY\_MOD::DO\_chemistry  
CHEMDR  
PHYSPROC  
CHEMISTRY\_MOD::GCKPP\_DRIVER  
GCKPP\_INTEGRATOR::INTEGRATE  
GCKPP\_INTEGRATOR::ROSENBROCK  
GCKPP\_INTEGRATOR::ROSENBROCK::ROS\_INTEGRATOR  
TRANSPORT\_MOD::DO\_TRANSPORT  
TRANSPORT\_MOD::GEOS4\_GEOS5\_GLOBAL\_ADV  
GCKPP\_INTEGRATOR::ROSENBROCK::ROS\_PREPAREMATRIX  
BPCH2\_MOD::READ\_BPCH2  
GCKPP\_INTEGRATOR::ROSENBROCK::ROS\_DECOMP  
GCKPP\_LINEARALGEBRA::KPPDECOMP  
EMISSIONS\_MOD::DO\_EMISSIONS  
STRAT\_CHEM\_MOD::DO\_STRAT\_CHEM  
STRAT\_CHEM\_MOD::GET\_RATES  
CALCRATE  
FAST\_J  
TPCORE\_FVDAS\_MOD::TPCORE\_FVDAS  
PHOTOJ  
JVALUE  
OPMIE  
OLSON\_LANDMAP\_MOD::COMPUTE\_OLSON\_LANDMAP  
MIESCT  
BLKSLV  
ISOROPIAII\_MOD::DO\_ISOROPIAII  
ISOROPIA  
ISRP3F  
VDIFF\_MOD::DO\_PBL\_MIX\_2



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7.908

7.904

.TAU application

GEOS\_CHEM

CHEMISTRY\_MOD::DO\_chemistry

CHEMDR

PHYSPROC

CHEMISTRY\_MOD::GCKPP\_DRIVER

GCKPP\_INTEGRATOR::INTEGRATE

GCKPP\_INTEGRATOR::ROSENROCK

GCKPP\_INTEGRATOR::ROSENROCK::ROS\_INTEGRATOR

TRANSPORT\_MOD::DO\_TRANSPORT

TRANSPORT\_MOD::GEOS4\_GEOS5\_GLOBAL\_ADV

42.786

24.235

GEOS\_CHEM

CHEMISTRY\_MOD::DO\_chemistry

3.677 GCKPP\_LINEARALGEBRA::KTF\_DECOM

3.026 EMISSIONS\_MOD::DO\_EMISSIONS

2.965 STRAT\_CHEM\_MOD::DO\_STRAT\_CHEM

2.853 STRAT\_CHEM\_MOD::GET\_RATES

2.268 CALCRATE

2.056 FAST\_J

1.902 TPCORE\_FVDAS\_MOD::TPCORE\_FVDAS

1.768 PHOTOJ

1.686 JVALUE

1.657 OPMIE

1.395 OLSON\_LANDMAP\_MOD::COMPUTE\_OLSON\_LANDMAP

1.292 MIESCT

1.279 BLKSLV

1.132 ISOROPIAII\_MOD::DO\_ISOROPIAII

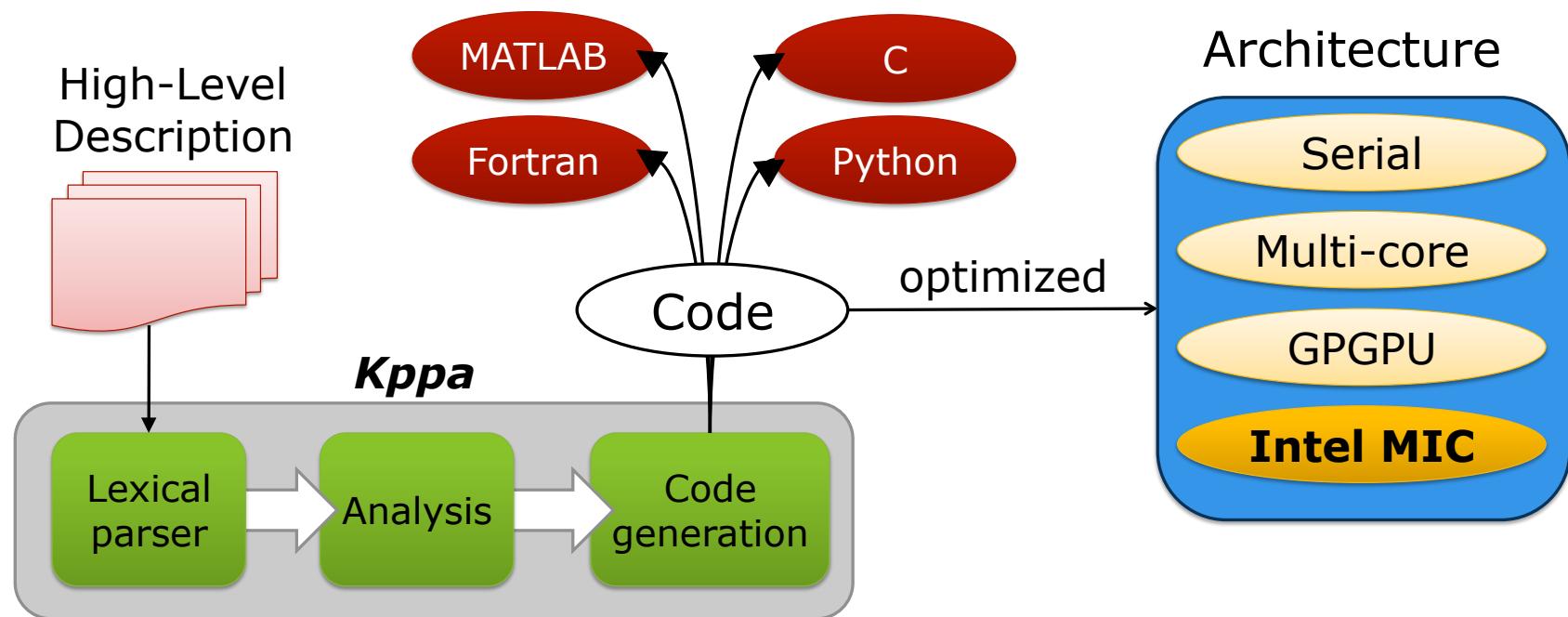
1.018 ISOROPIA

0.99 ISRP3F

0.964 VDIFF\_MOD::DO\_PBL\_MIX\_2

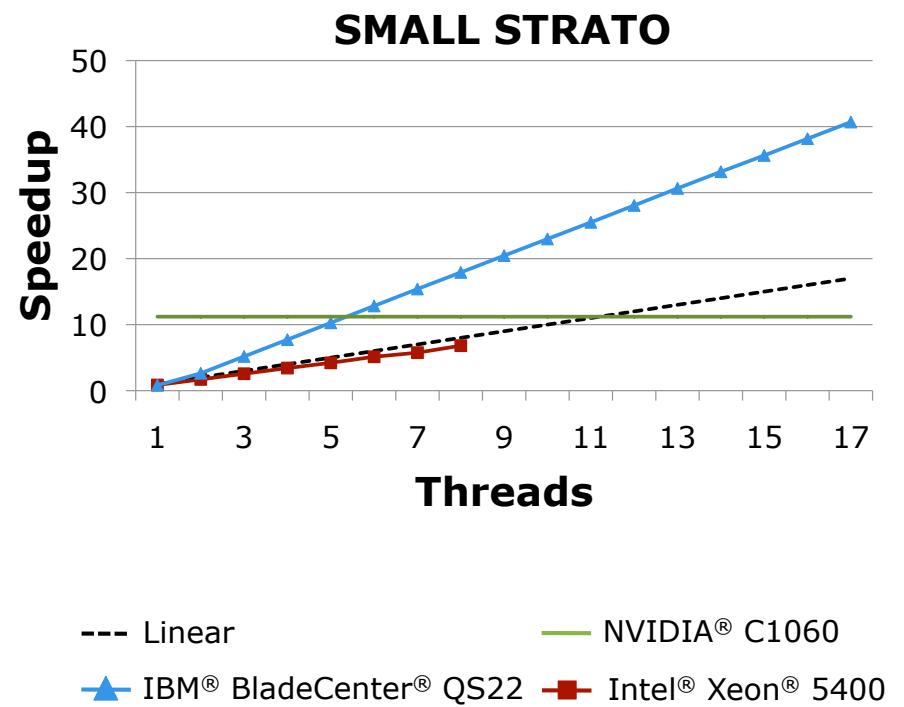
Twelve Threads  
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# Kppa: The Kinetic PreProcessor Accelerated



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

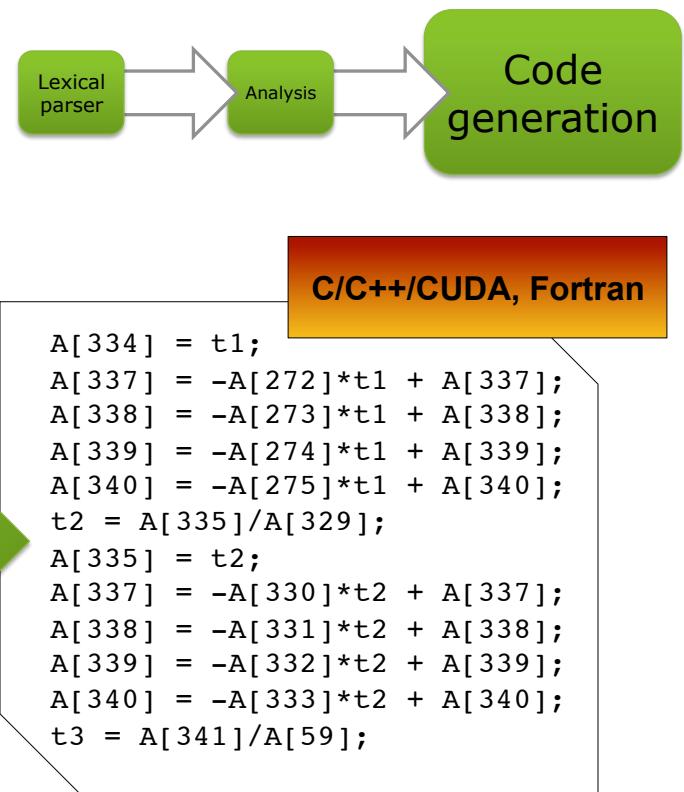
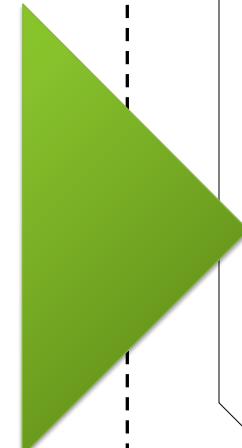
- Reorder chemical species to **minimize fill-in**
- Reorder concentration data to **maximize vectorization**
- Reorder grid cells to **reduce excessive iteration**



# Meta-programming for Automatic Code Generation

```
<%
d_Decomposition.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_Decomposition.end() %>
```



# Kppa's Architecture Parameterization

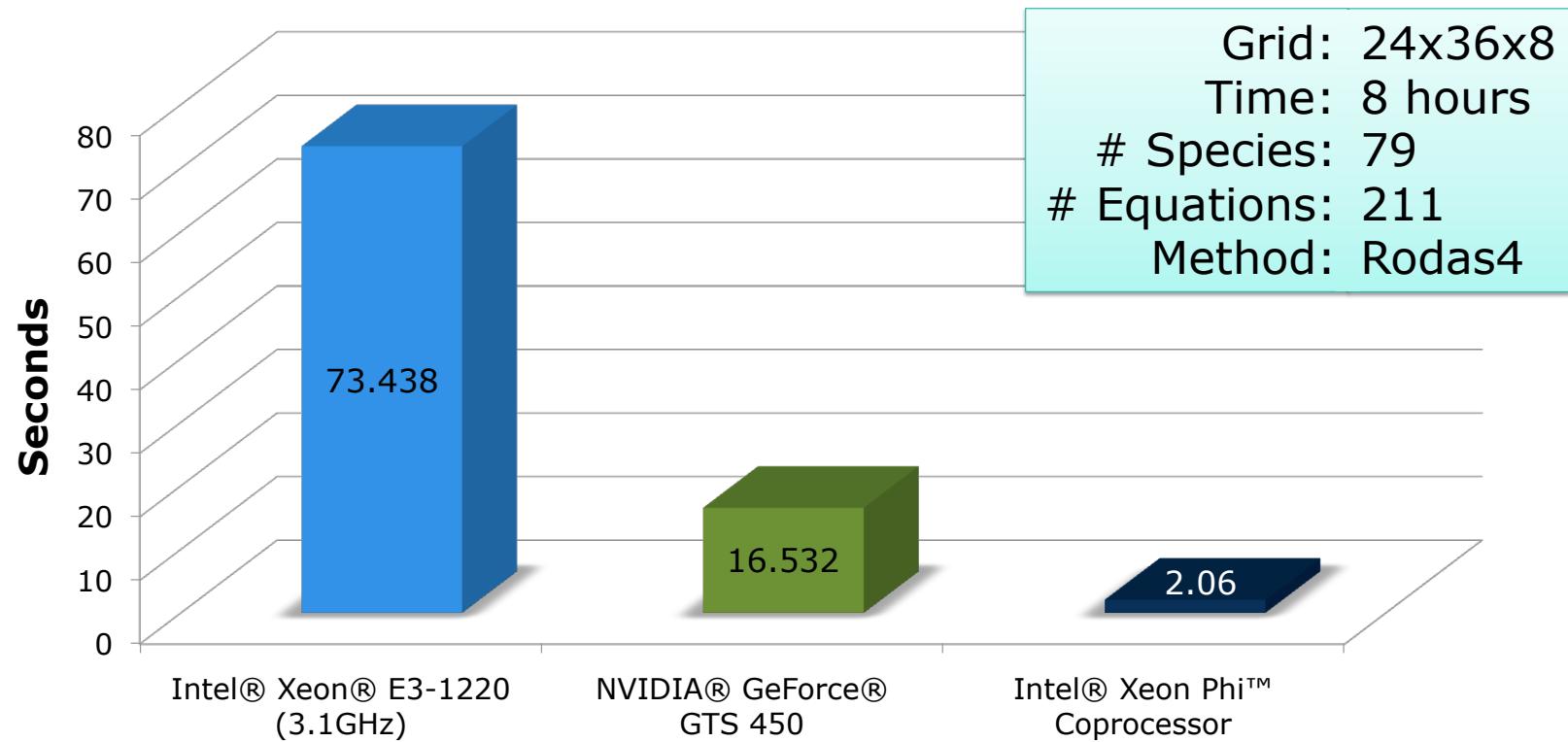
	CPU	GPU	Intel® MIC	CBEA
<b>Instruction Cardinality</b>	1	32	16	4
<b>Integrator Cardinality</b>	1	$\infty$	16	4
<b>Scratch Size</b>	N/A	16 KB	N/A	256 KB

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

Targeting the Intel® Xeon® Phi™ coprocessor was easy!



## Kppa-generated SAPRC Kernel: 35.6x Speedup





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

Paratools