High Performance Computing on CTU Prague

Dr. Petr Pospisil

pospisil@vc.cvut.cz

Computing and Information Centre
Czech Technical University in Prague

Prague, Czech Republic

1. Part

High Performance Computing on CTU Prague

- list of projects solved on Altix (2004 – 2005)

2. Part

„Bandwidth Challenge“ on Altix

- talk during Supercomputing05 (SGI booth)

Hardware

- **SGI Altix 3700**

  16 x 1.3 GHz Intel Itanium 2 , 3MB L3 cache

  8 x 1.5 GHz Intel Itanium 2, 6MB L3 cache

  64 GB global shared memory

- **IBM SP, 40 cpus Power3, 18 GB RAM**

Software

Propack 3.0 , Linux Red Hat

Intel compilers 8.0, MKL 7.2

Applications:

Gaussian03, Fluent 6.2.16, Abaqus 6, Mathematica 5.2, PETSc

Debugger: **Totalview**

Batch system: **PBSpro**

Institutions

Czech Technical University, Prague

Institute of Chemical Technolog

University of J. E.

University of Ostrav

Academy of Sc

Charles University, Prague

Department of Physics

Facult Engineering

Department of Organic Chemistry

ing

Department of Physics, Faculty of Science

Institute of Atmospheric Physics
Institute od Chemical Process Fundamentals
Institute of Macromolecular Chemistry

ramics

Department of Macromolecular Physics
Faculty of Mathematics and Physics

stitute of Experimental and Applied Physics

Faculty of Civil Engineering CTU

Department of Irrigation, Drainage and Landscape Engineering

1 **Simulation of Flow and Transport in Vadose Zone**

FEM (and PETSc) is used to solve Richard´s equation in two or three dimensions. Richard´s equation is commonly used for the modelling the flow in the unsaturated porous media.

-Highly demanding as to HPC

-LRZ Munich (new big Altix is being built)

Dep

2 **Tun**

Faculty of Civil Engineering CTU

Department of Irrigation, Drainage and Landscape Engineering

1 **Simulation of Flow and Transport in Vadose Zone**

TFS is studied after excavation before steel lining

Department of Structural Mechanics

2 **Tunnel Face Stability**

Ing. Martin J. Valek Ph.D

Faculty of Mechanical Engineering CTU

Departme

ABAQUS

3 Temperature-stress analysis of big diesel engine cylinder head

Ing. Miroslav Spaniel, CSc., Ing. Radek

rcel Divis

FLUENT

Department o luid Dynamics and Power Engineering

4 Modelling of Internal Fluid Flow in Brown Coal Mill Loop

FLUENT, Diploma thesis

5 Car side windows soiling simulation

J. Klimes

Department of Environmental Engineering

6 **Temperature distribution in car interior**

Sponiar David, Ing. Martin Bartak

7 **CFD Simulation of indoor environment in buildings under real outdoor conditions**

Ing. Bartak

FLUENT

Depa

PETSc is used to solve turbulent fluxes in complex geometries

8 **Numerical solution of compressible flows on unstructured meshes**

Ing. Jiri Dobes

9 **Numerical methods for solution of transonic flows**

-finite element volumes are used

Center for Aerospa

Compressor for aircraft engine

10 **First stage of the centrifugal compressor design with tandem rotor blades**

Ing. T. Censky

Research Center of Applied Cybernetics

11 **Mathematical modelling of electron transport during photosynthesis**

Ing. Cerveny

Faculty of Electrical

Department of Physics

-Magneto-hydrodynamics
-Astrophysical plasma

12 **CFD Data Visualisation**

Ing. D. Skandera

13 **Nonlinear sound interactions in acoustic resonators**

Ing. Milan Cervenka, PhD

14 **Numerical solving of Burger's type equations**

M. Marcicovsky

Department of Control Engineering

15 **Polynomial matrix computation in Mathematica**

Ing. Kujan

Department of Computer Science and Engineering

16 **Parallel algorith**

-data mining

-artificial intelligence

17 **Parallel and sequential derivation of association rules**

Robert Kessl

Department of Cybernetics

18 **Randomized distributed search methods for large state spaces**

Ing. Filip Zelezny, PhD

Faculty of Nuclear Sciences and Physical Engineering CTU

Department of Materials

ABAQUS

19 **Stress-strain field computations in fracture mechanics specimens**

Dr. Ing. Petr Hausild

Department of Mathematics

20 **Parallel algorithms for solution of nonlinear partial differential equations**

Dr. Ing. Michal Benes, Ing. Zdenek

-microstructures in materials
-contamination transport in air
-population dynamics

21 **Applicat**
mathema

Ing. Severin Posta, PhD

Departr

-light propagation
-diffusive processes modeling

22 **Research centre for optics**

Mgr. Natalyia Tarasenko; Prof. Ing. Zdenek Bryknar, CSc. ; RNDr. Lubomir Jastrabik, CSc

Department o

-fractures in iron crystals

23 **Atomic simulation of physical properties of bcc Fe**

-material diagnostics

-construction defectoscopy

24 **Elastic waves propagation in arbitrary inhomogeneous media**

-catalytic effect of the clusters is studied

25 **DFT study of the interaction of organic molecules with gold and platinum clusters**

J.Sebera, Ing. Zalis

Fac

Dep

Very detailed FEM methods of human muscular-skeletal system will be created to be able to analyze different car crash injuries

26 **FE models in biomechanics constructed using computer tomography data**

Ing. Ondrej Jirousek

Departm

Nonlinear effects which arise in the stimulated Raman scattering are studied

27 **Nonlinear effects study in plasma physics**

RNDr. Zuzana Mala, PhD

Institute of Experimental and Applied Physics CTU

Department of Theory and Modeling

28 ATLAS is detector of radioactivity, which is being built in CERN -part of LHC

ATLAS

29 **Study of the production of top-antitop quark pairs in the experiment ATLAS**

Ing. Karel Smolek

Insti

Relationship between structure and reactivity of organic materials is studied

Depar

30 **Stud**

FLUENT is used to compute velocity fields, profiles of concentration, …

Department of C… …l Engineering

31 **Simulations of multiphase flows in stirred systems**

Density functional theory (DFT) simulations are used

Departm

32 **Influence of nitrogen on the structure and properties of silicate glass**

Ing. Jan Machacek

Universit

Departm

Several mechanisms of nanochemical elements are studied

33 **Molecular simulation of nanochemical elements**

Nano-configuration impacts are studied
-on chemical reactions
-on reactive kinetics

34 **Molec**
linear

35 **Molecular-level simulation study of chemical mixtures in nanoporous materials**

Mgr. J. Krejci

Acad

Institu

IAF and KAMM models are used to simulate air and temperature fluxes

36 **Modelling of wind fields over Ore mountains and Prague**

RNDr. Jaroslav Svoboda CSc., Mgr. Jiri Hosek

In

Hydrodynamics of multiphase systems:
Gas – liquid
Liquid – solid substance

37 **id**

38 **Computer simulation of the multiphase systems hydrodynamics**

Ing. Jiri Kristal

University of Ostrava

Department

39 **Structu cluster i**

40 **Fragme Rare** **s**

Standard methods of physical chemistry is used
(Born-Oppenheimer approximation, Diatomics-in-molecules method)
Hen+, Arn+, Krn+, Xen+

41 **Theoretical exploration of the rare gas cations**

Mgr. Daniel Hrivnak

Charles University, Prague

Dep
Facu

Diploma thesis under guidance of
Prof. S. Nespurek
(Institute of Macromolecular Chemistry
Academy of Sciences, Prague)

42

Po
pa

J. Nozar

END

of 1. Part

„Bandwidth Challenge“ on Altix

Dr. Petr Pospisil

pospisil@vc.cvut.cz

Computing and Information Centre
Czech Technical University in Prague

Prague, Czech Republic

Memory bandwidth benchmark

STREAM

John McCalpin
www.cs.virginia.edu/stream/

Designed for SMP machines

STREAM2

vector copying

1. Self-programmed code

STREAM

2. Library function dcopy from MKL, SCSL

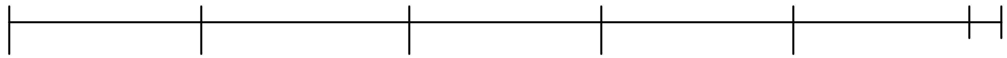
Parallel copying of vector Y[0:N] into vector X[0:N]

OMP_NUM_THREADS = ***nthreads***

C - code

```
#pragma omp parallel for
    for(i=0; i<N;i++)
        X[i]=Y[i];
```

Library: cblas_dcopy(N,X,1,Y,1) & domain decomposition



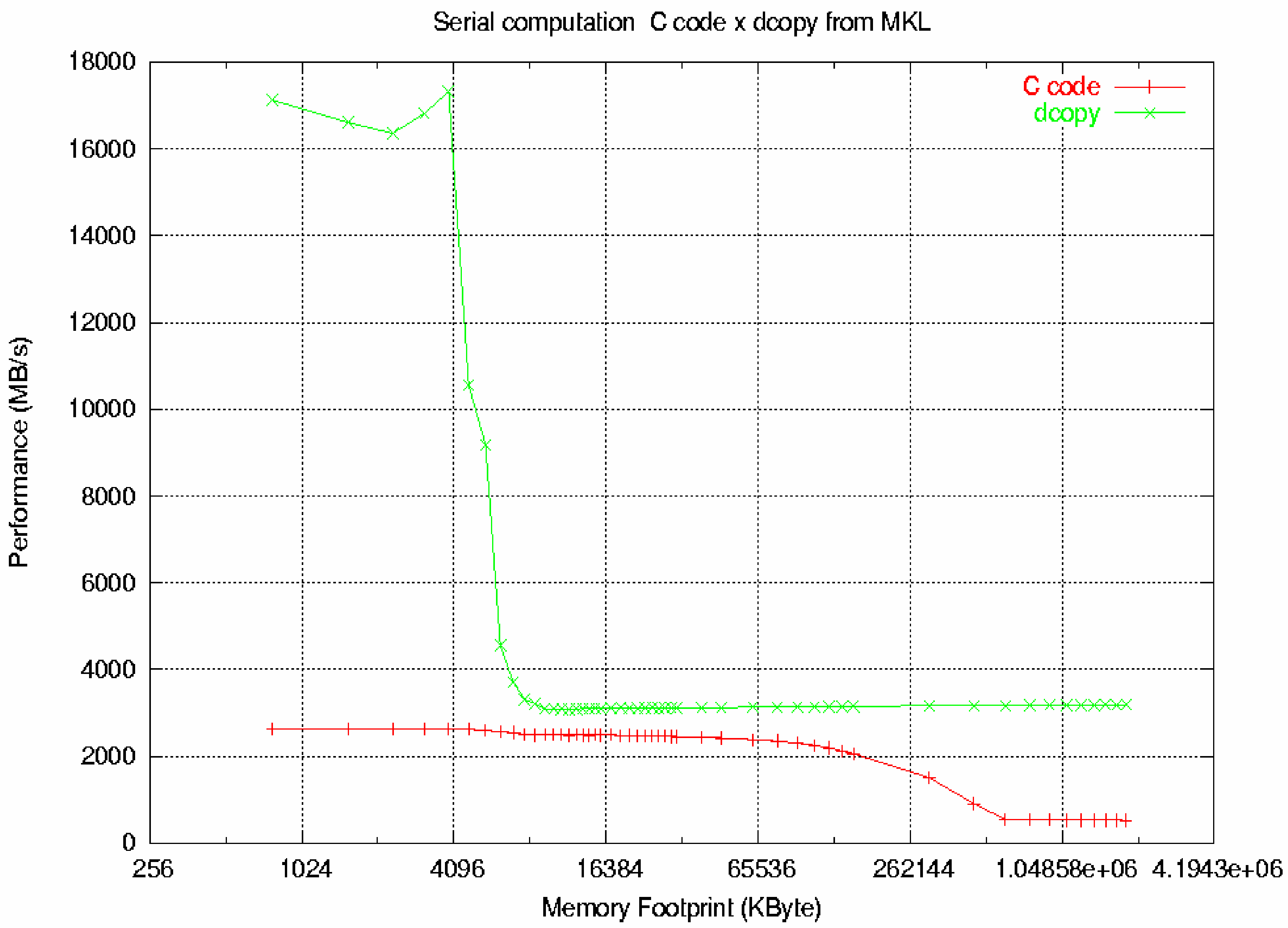
```
#pragma omp parallel for
    for(i=0; i<nthreads; i++)
(void) cblas_dcopy(N/ nthreads, X + N/ nthreads * i, 1,
                       Y + N/ nthreads * i,1);
```

Intel compiler for Linux: icc with commands -O3 -openmp

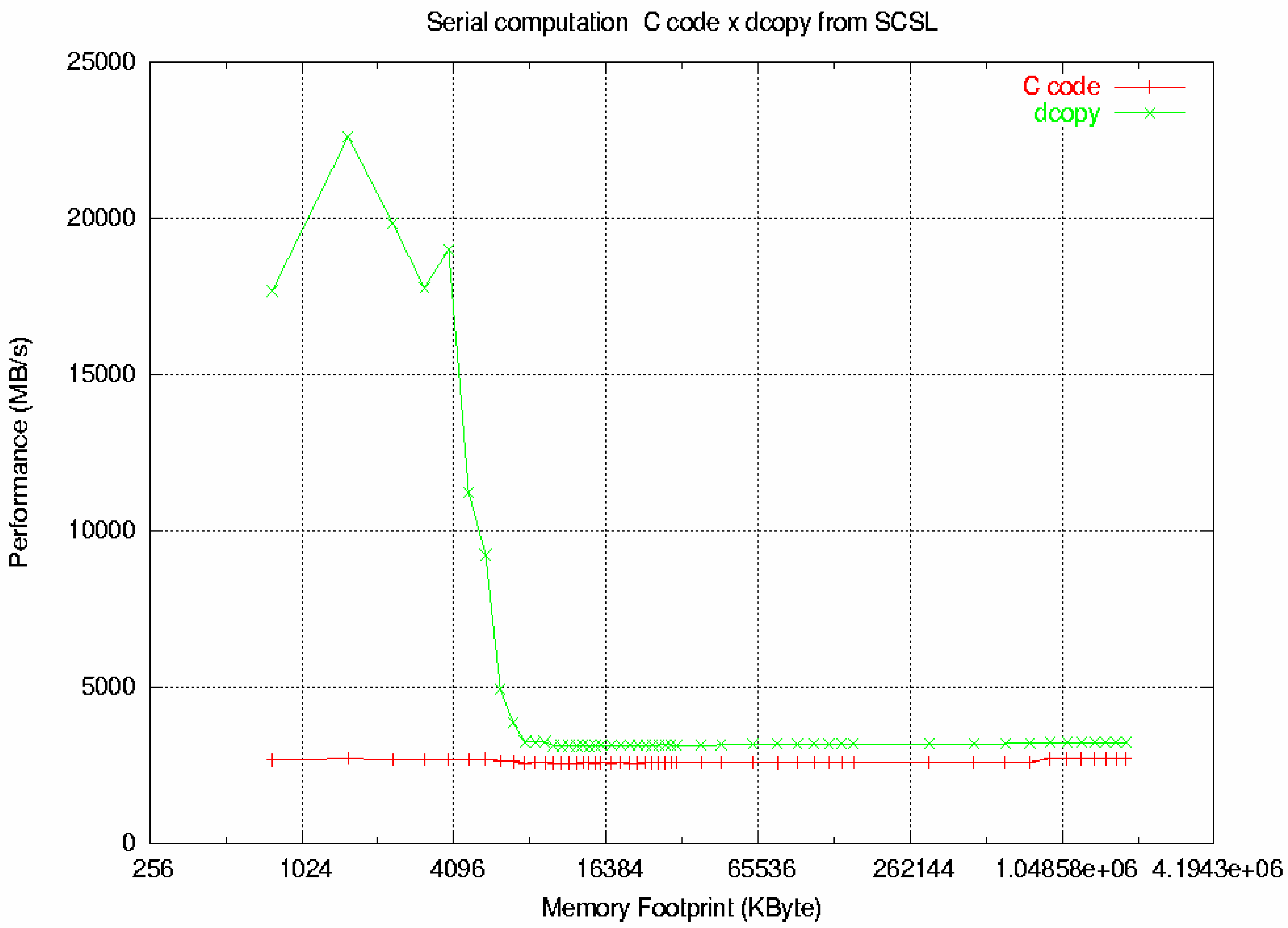
Serial computation performance !!

Prof. Stout: Doubling serial performances far more useful than doubling the number of processors

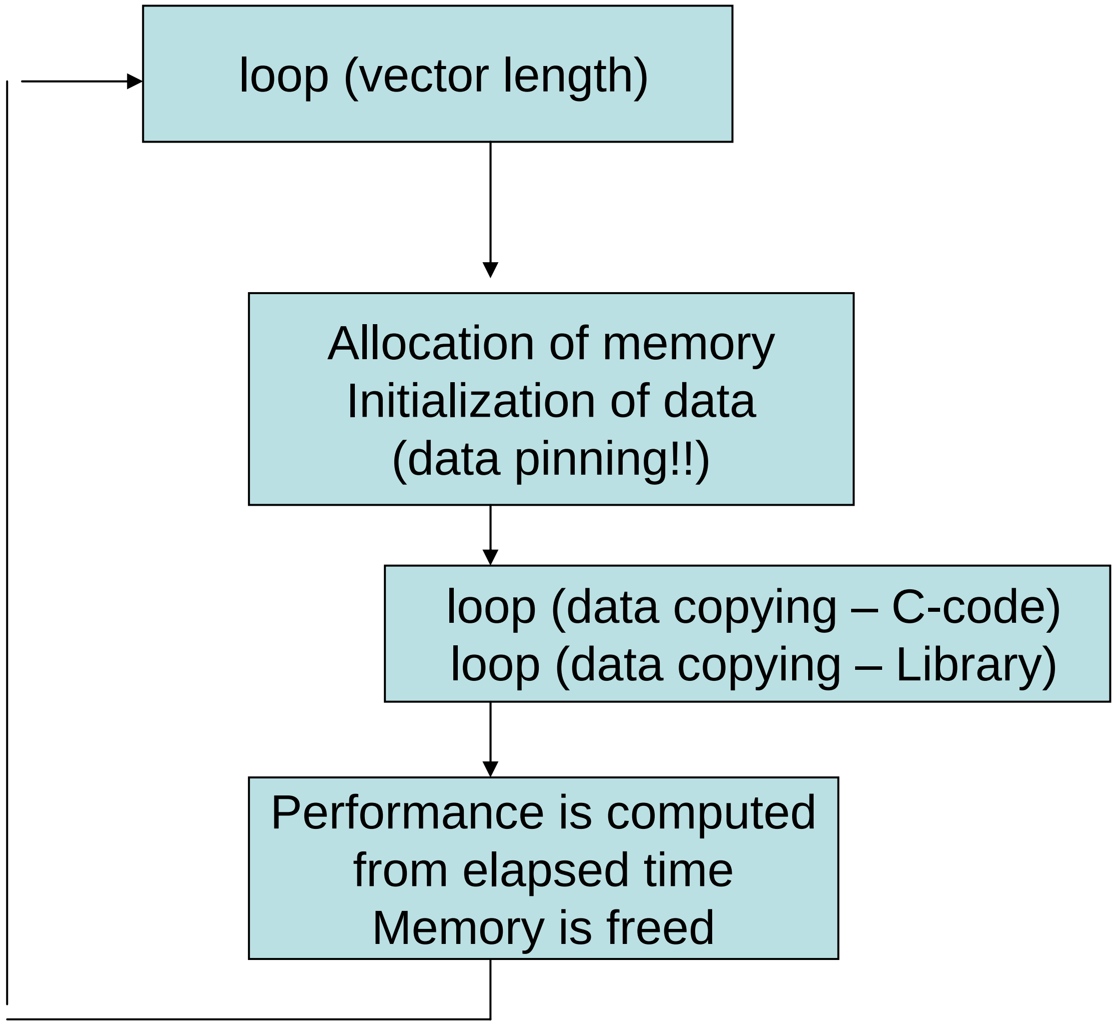
OMP_NUM_THREADS = 1



Serial computation C code x dcopy from MKL
C code
dcopy
Performance (MB/s)
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)


Serial computation C code x dcopy from SCSL
C code
dcopy
Performance (MB/s)
25000
20000
15000
10000
5000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)

Program organization

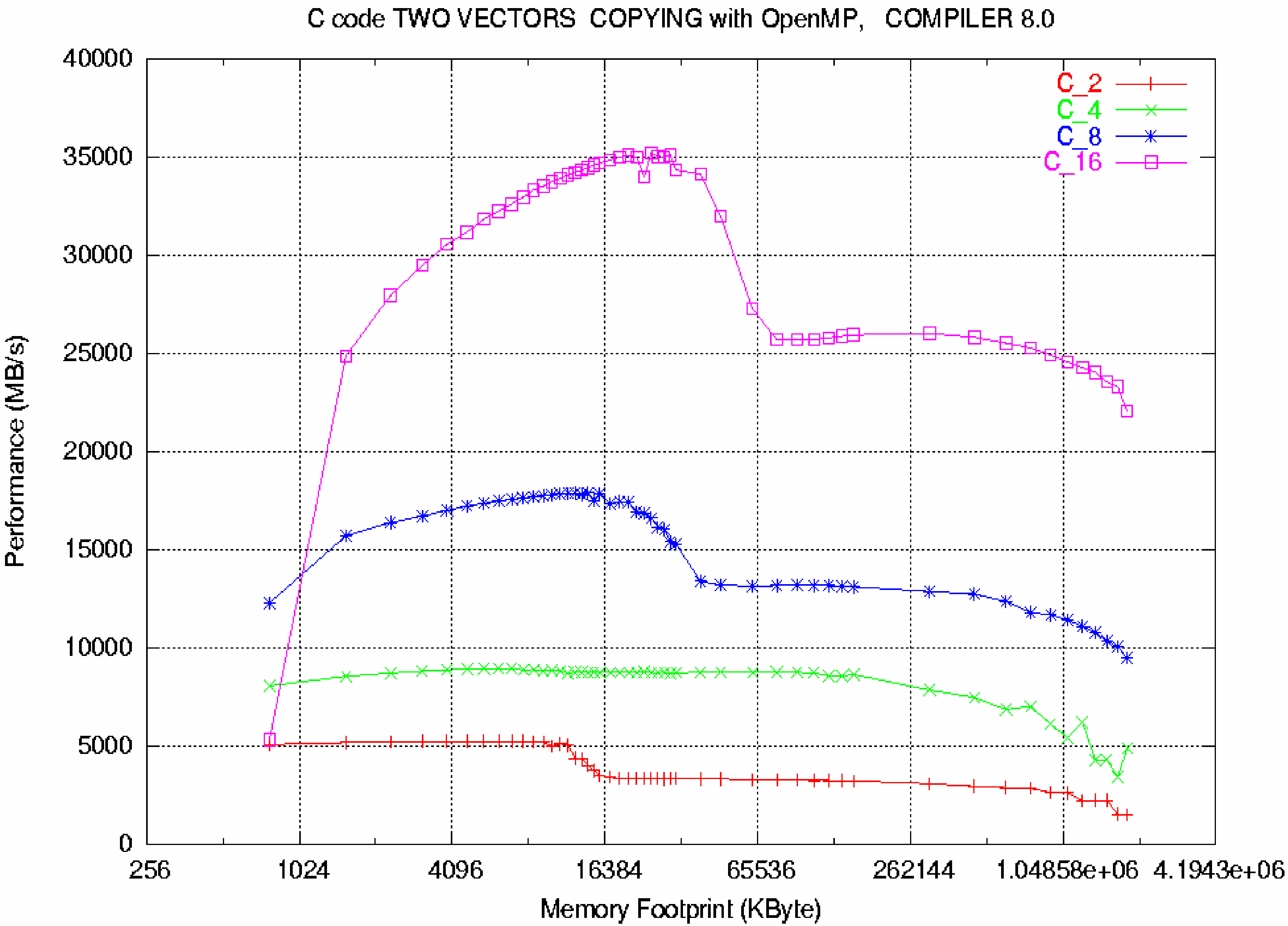


Computers:

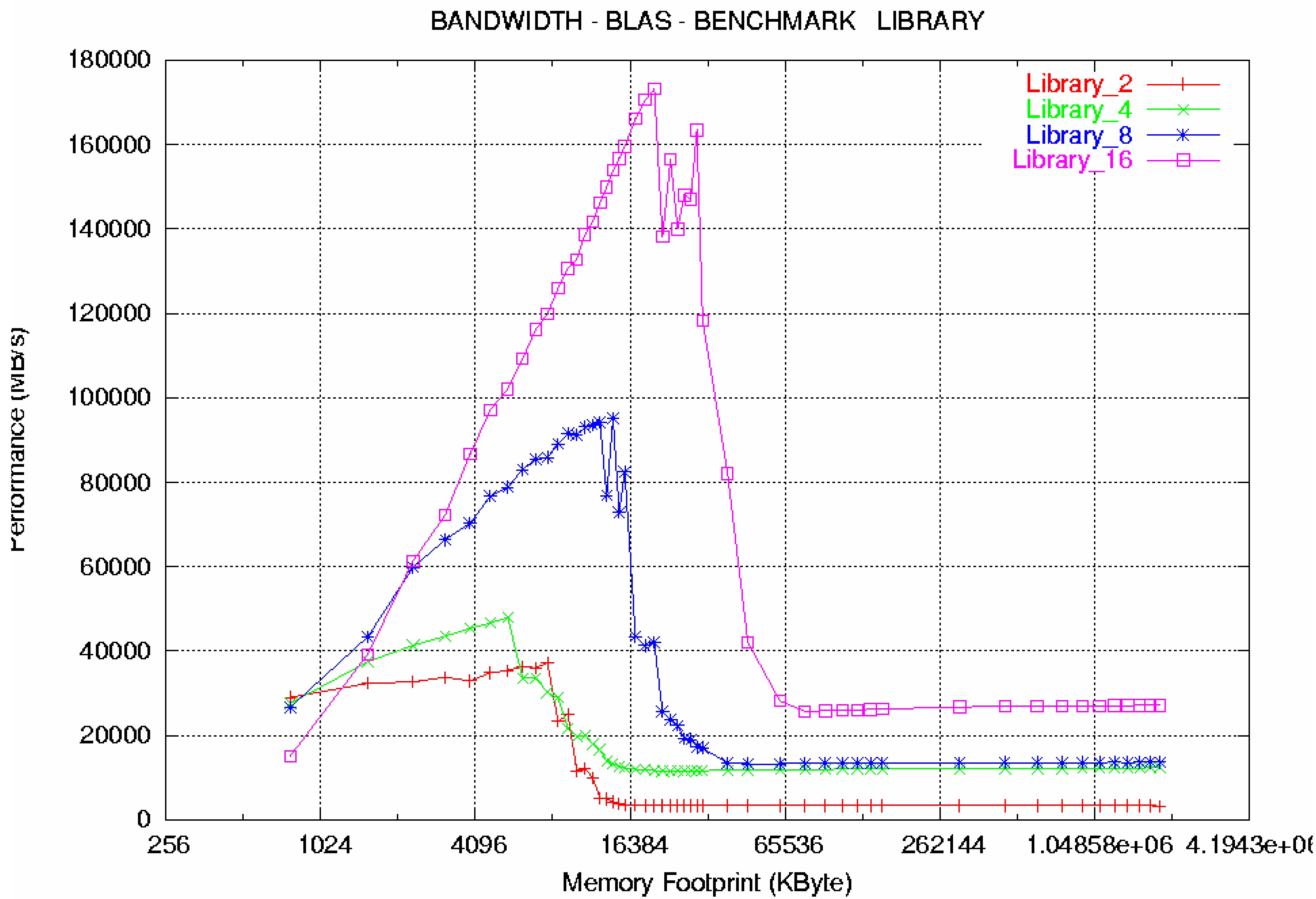
our Altix, 24 CPUs, 1.3 GHz, 3MB L3 cache

Mountain View

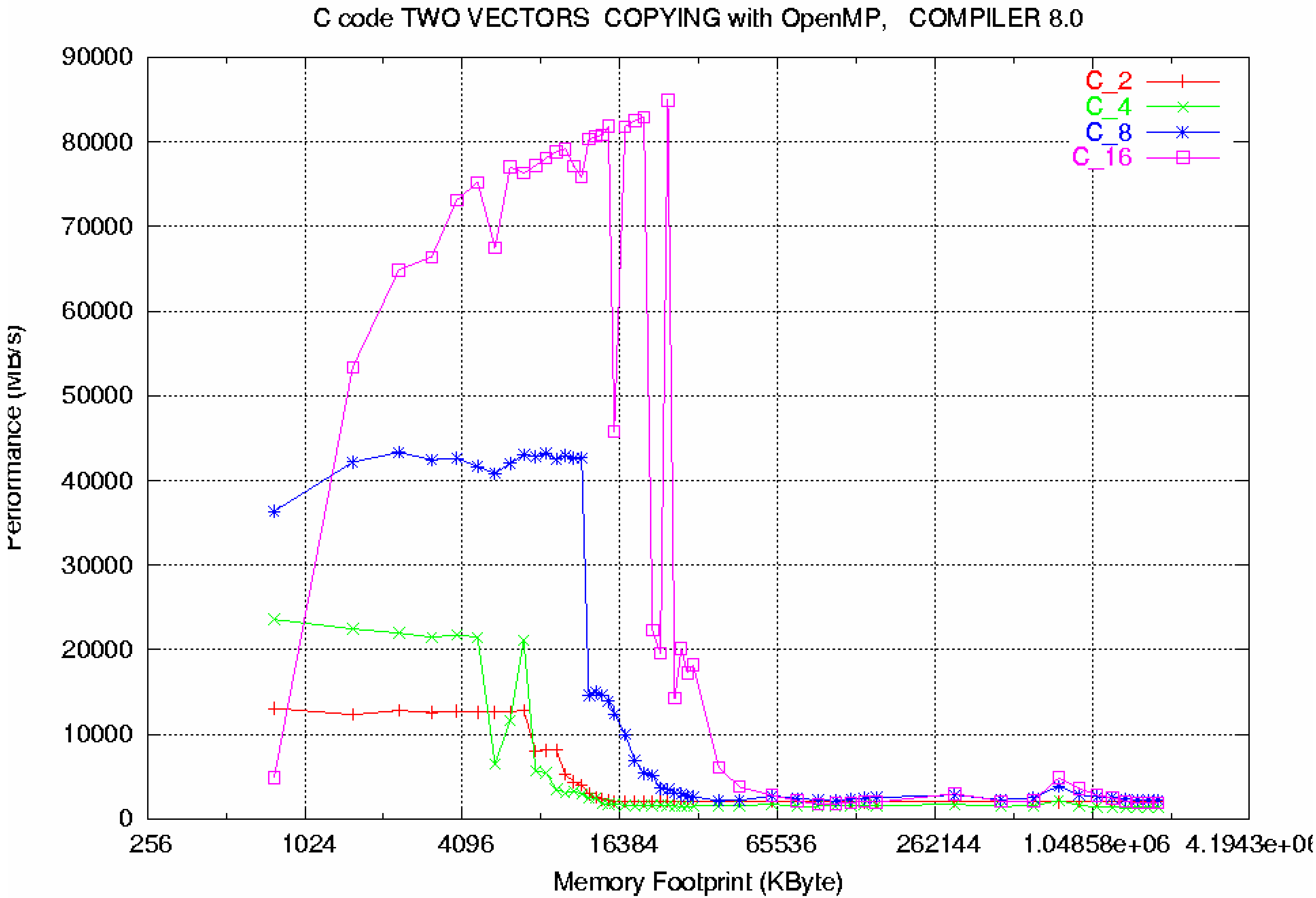
Altix 3700 Bx2, 128 CPUs, 1.6GHz, 9 MB L3 cache


C code TWO VECTORS COPYING with OpenMP, COMPILER 8.0
C_2
C_4
C_8
C_16
Performance (MB/s)
40000
35000
30000
25000
20000
15000
10000
5000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)

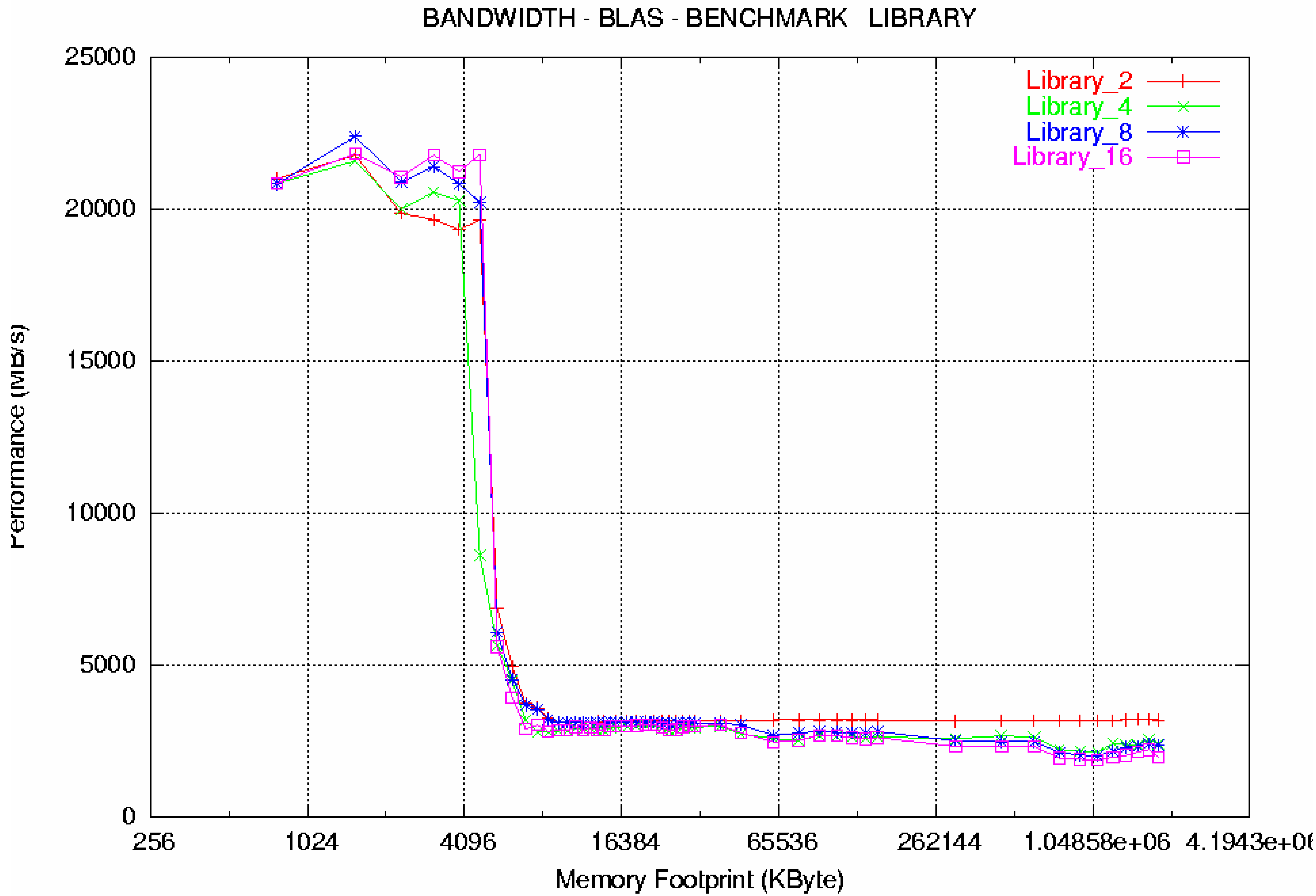
MKL library

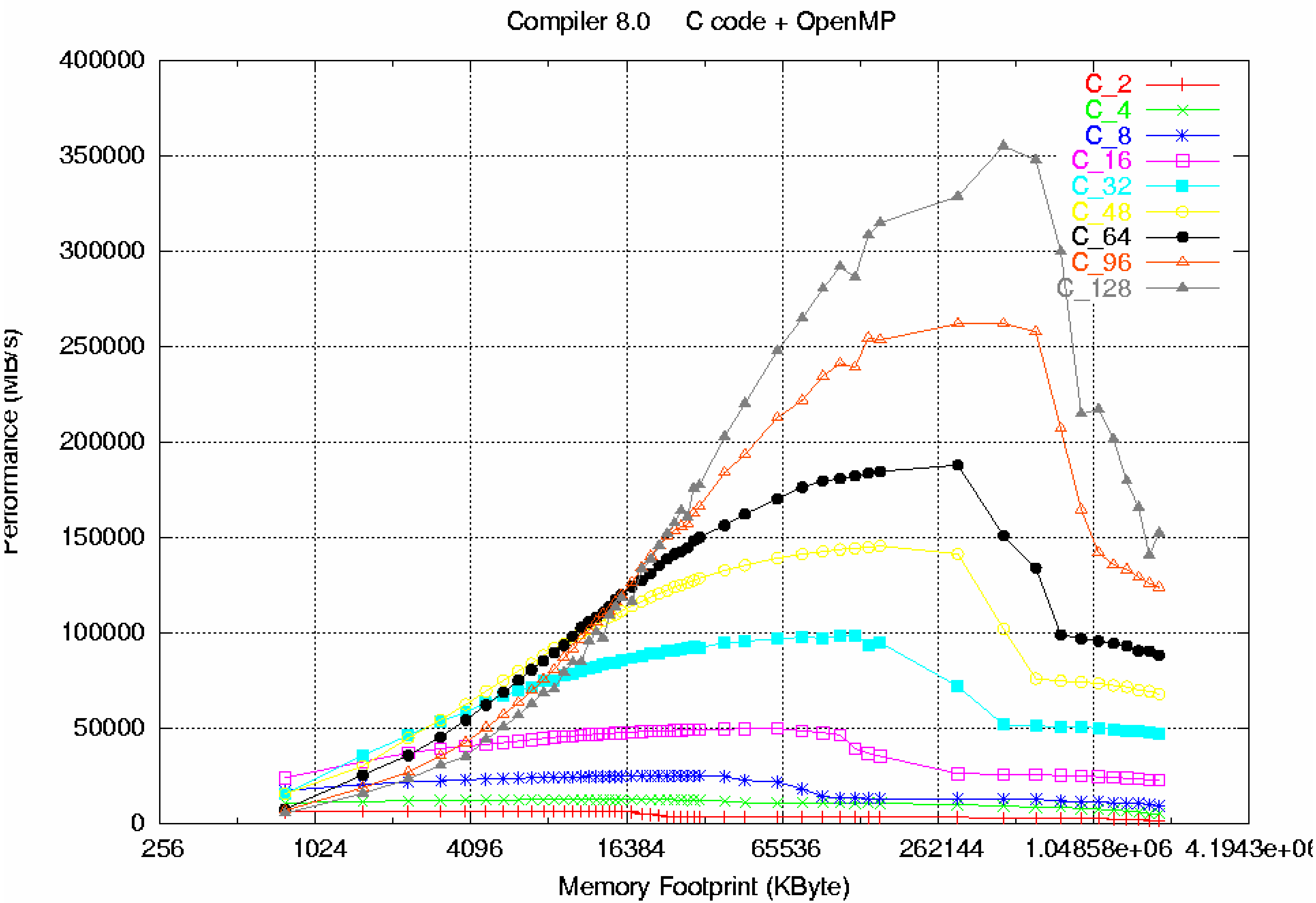

BANDWIDTH - BLAS - BENCHMARK LIBRARY
Performance (MB/s)
Memory Footprint (KByte)
Library_2
Library_4
Library_8
Library_16
0
20000
40000
60000
80000
100000
120000
140000
160000
180000
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06

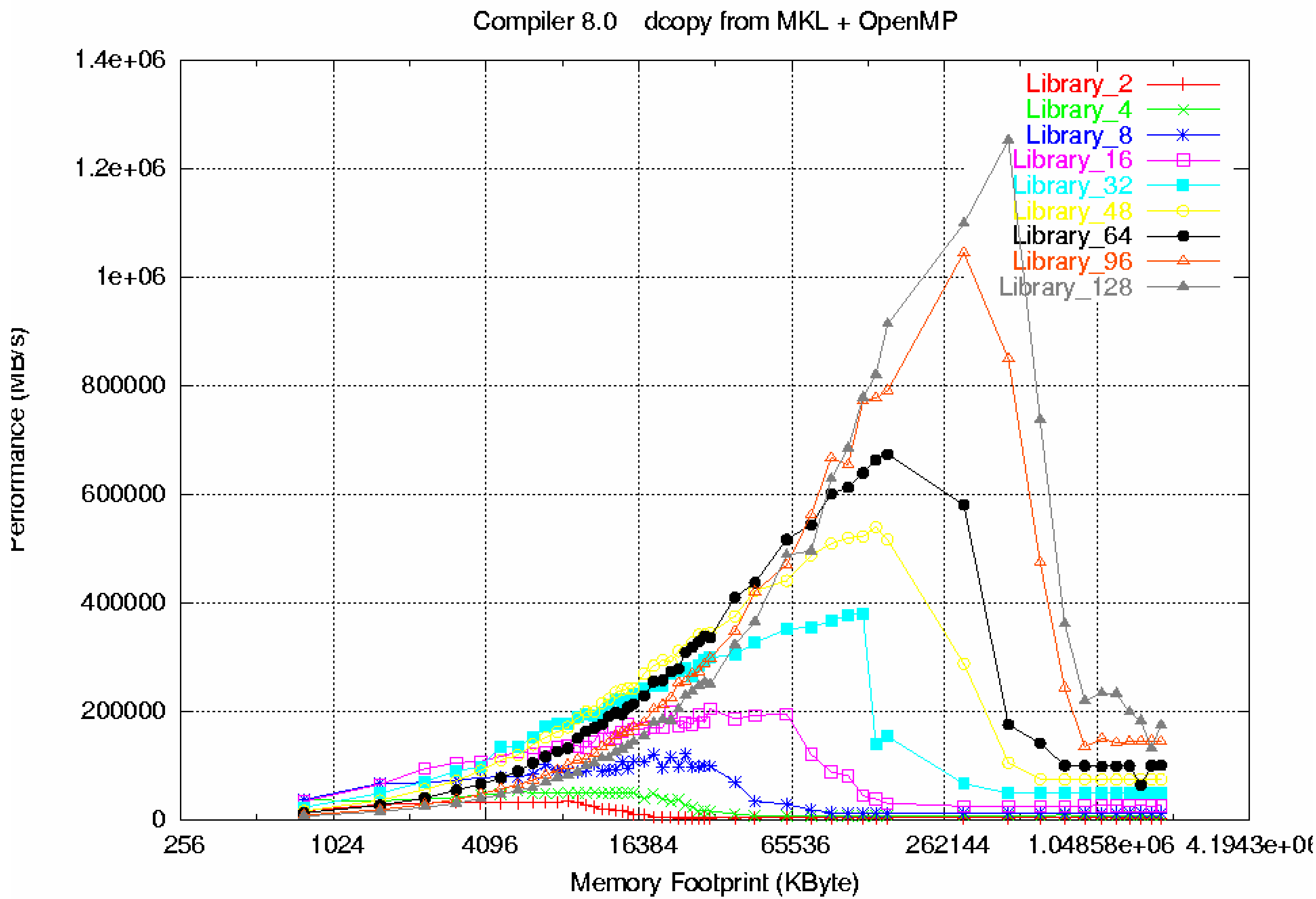
SCSL library



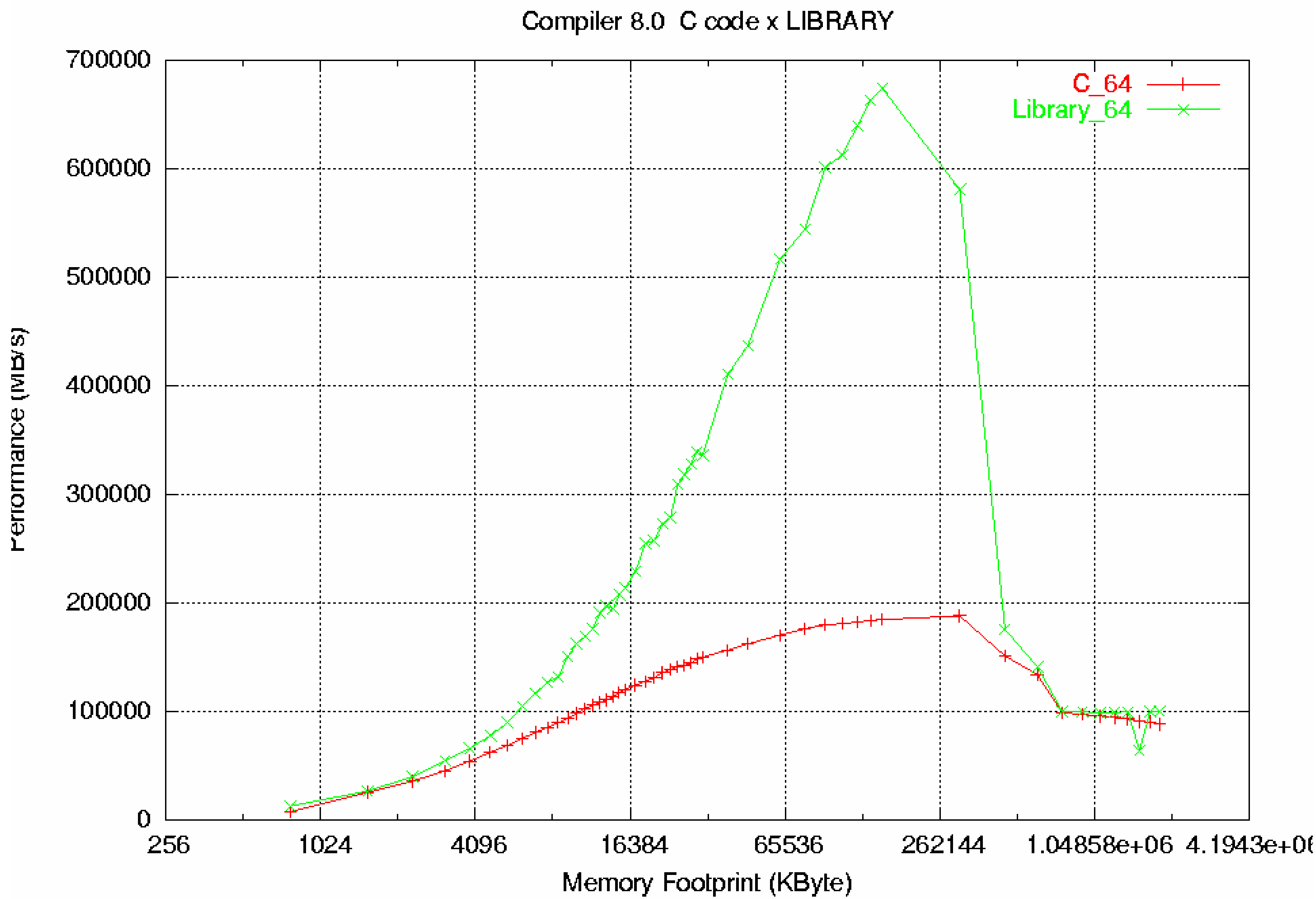
SCSL library

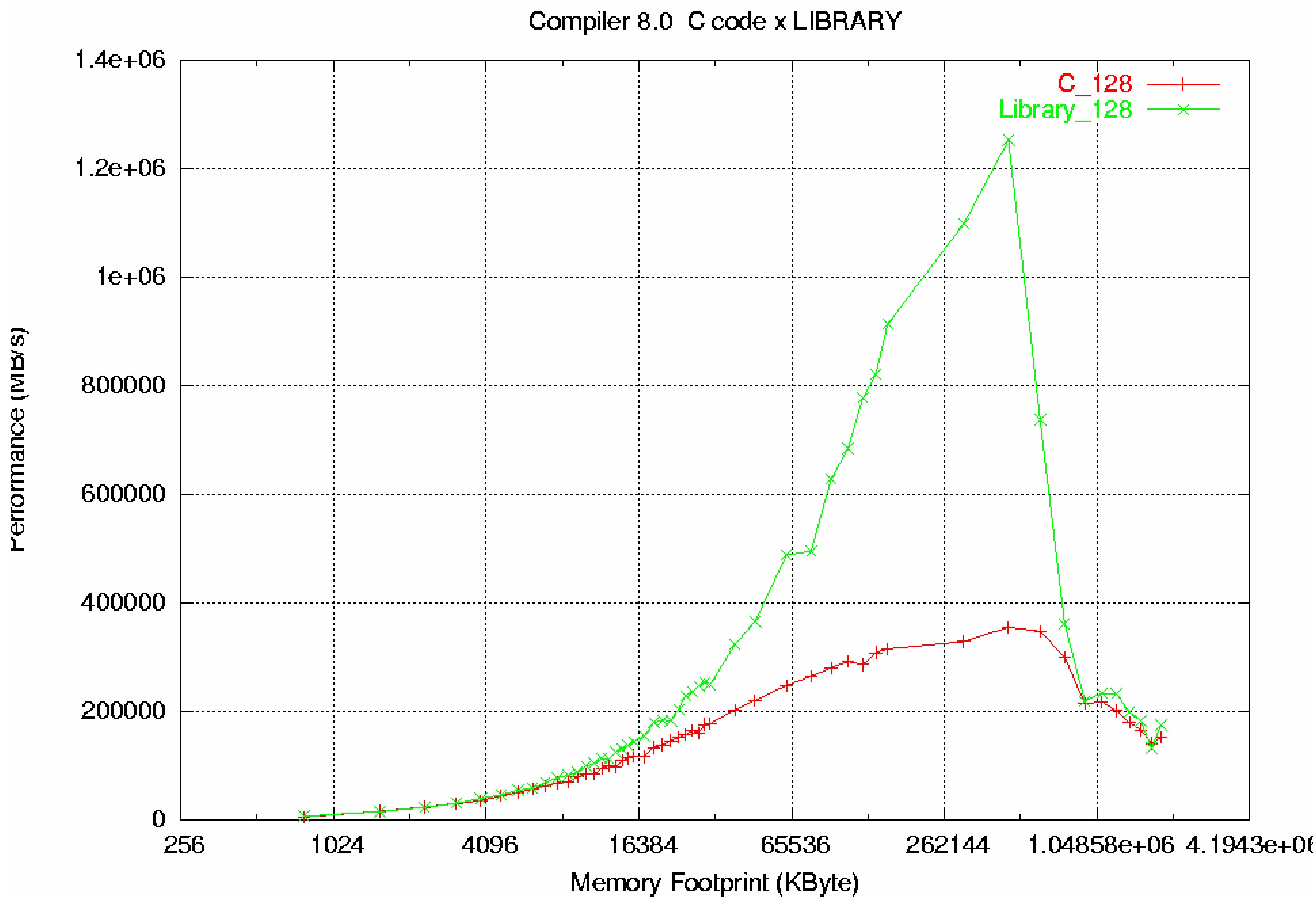


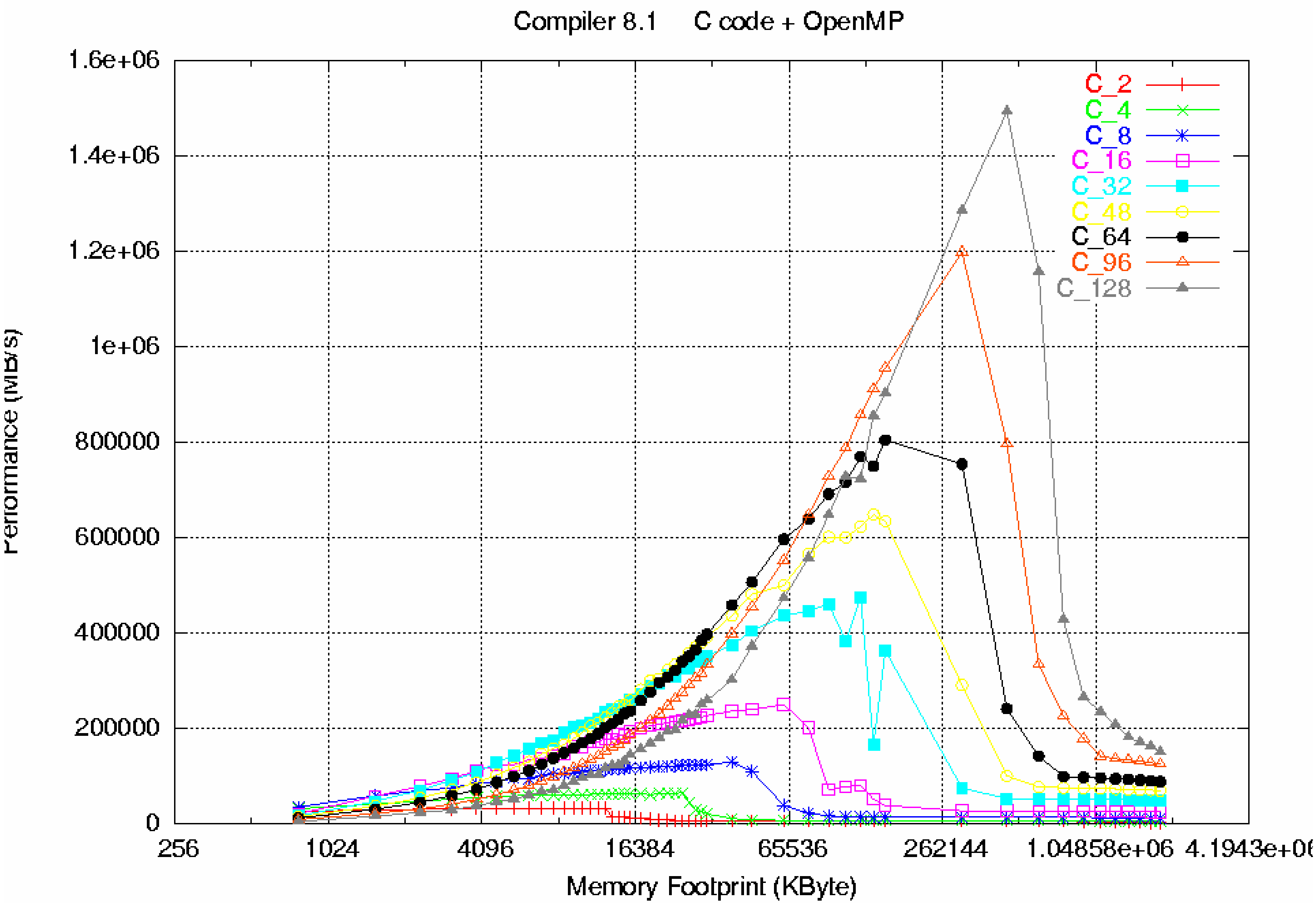

Compiler 8.0 C code + OpenMP
Performance (MB/s)
Memory Footprint (KByte)
400000
350000
300000
250000
200000
150000
100000
50000
0
256
1024
4096
16384
65536
262144
1.04858e+06
C_2
C_4
C_8
C_16
C_32
C_48
C_64
C_96
C_128

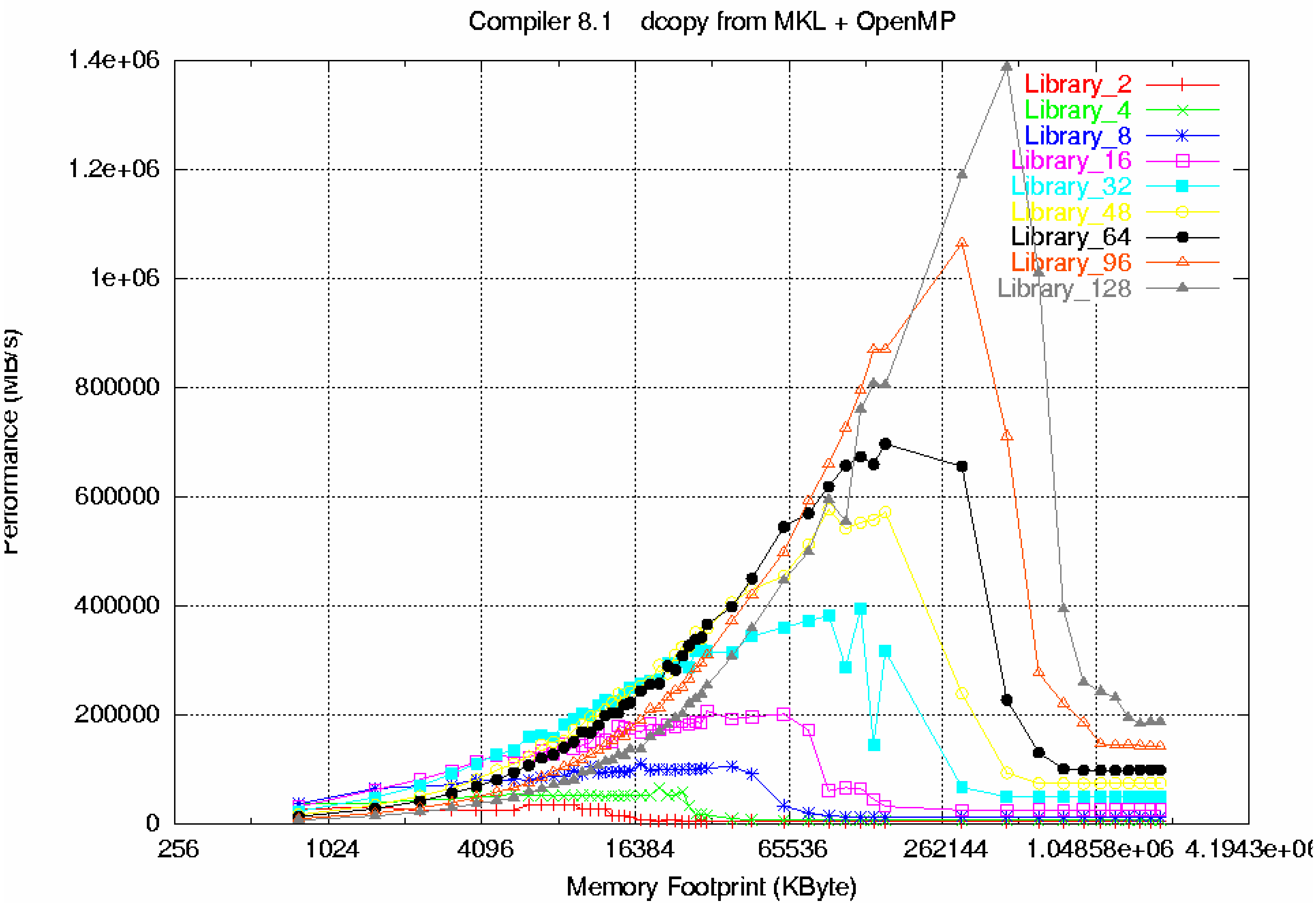


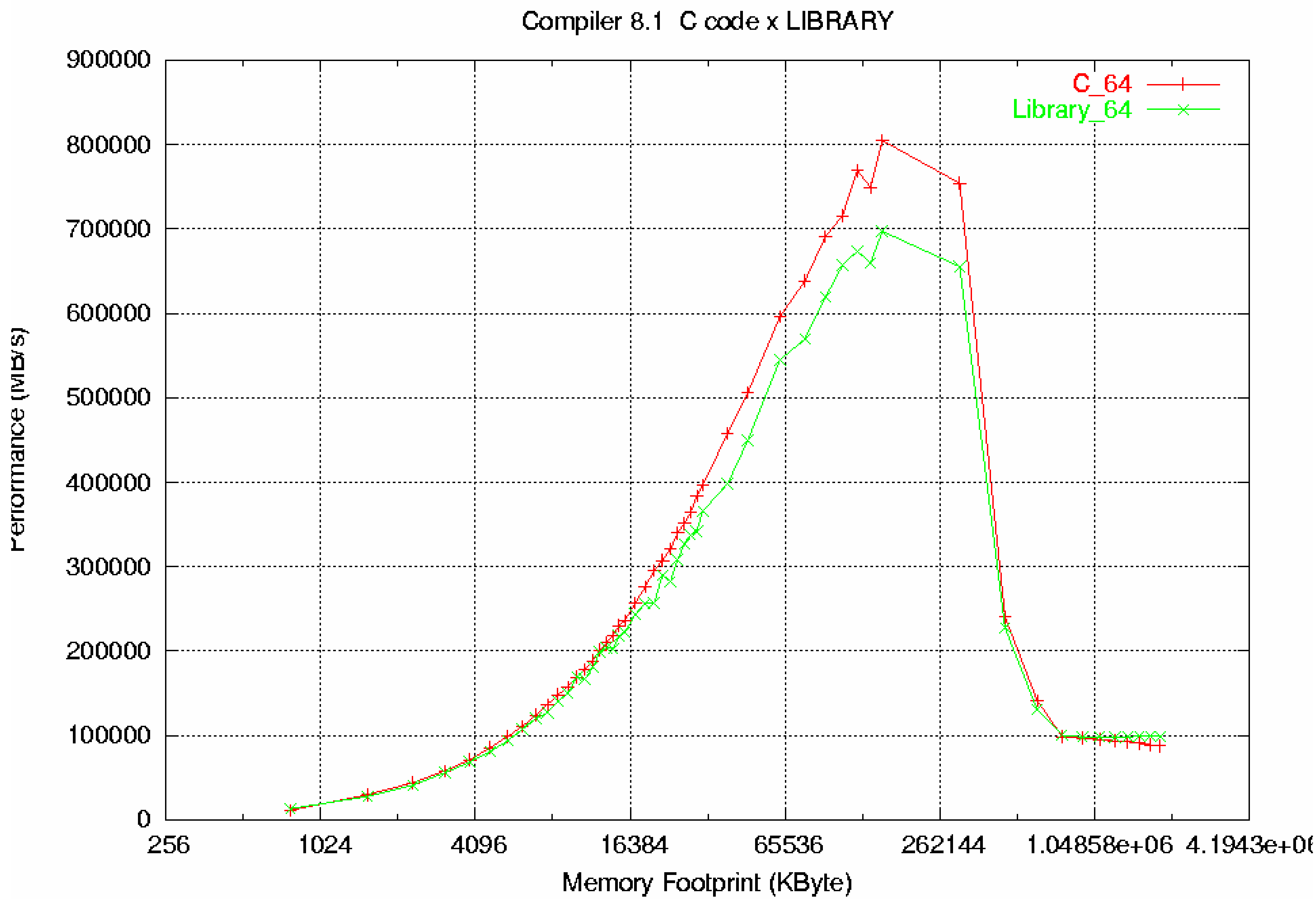
Compiler 8.0 dcopy from MKL + OpenMP
Performance (MB/s)
Memory Footprint (KByte)
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
Library_2
Library_4
Library_8
Library_16
Library_32
Library_48
Library_64
Library_96
Library_128


Compiler 8.0 C code x LIBRARY
Performance (MB/s)
Memory Footprint (KByte)
C_64
Library_64
0
100000
200000
300000
400000
500000
600000
700000
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06

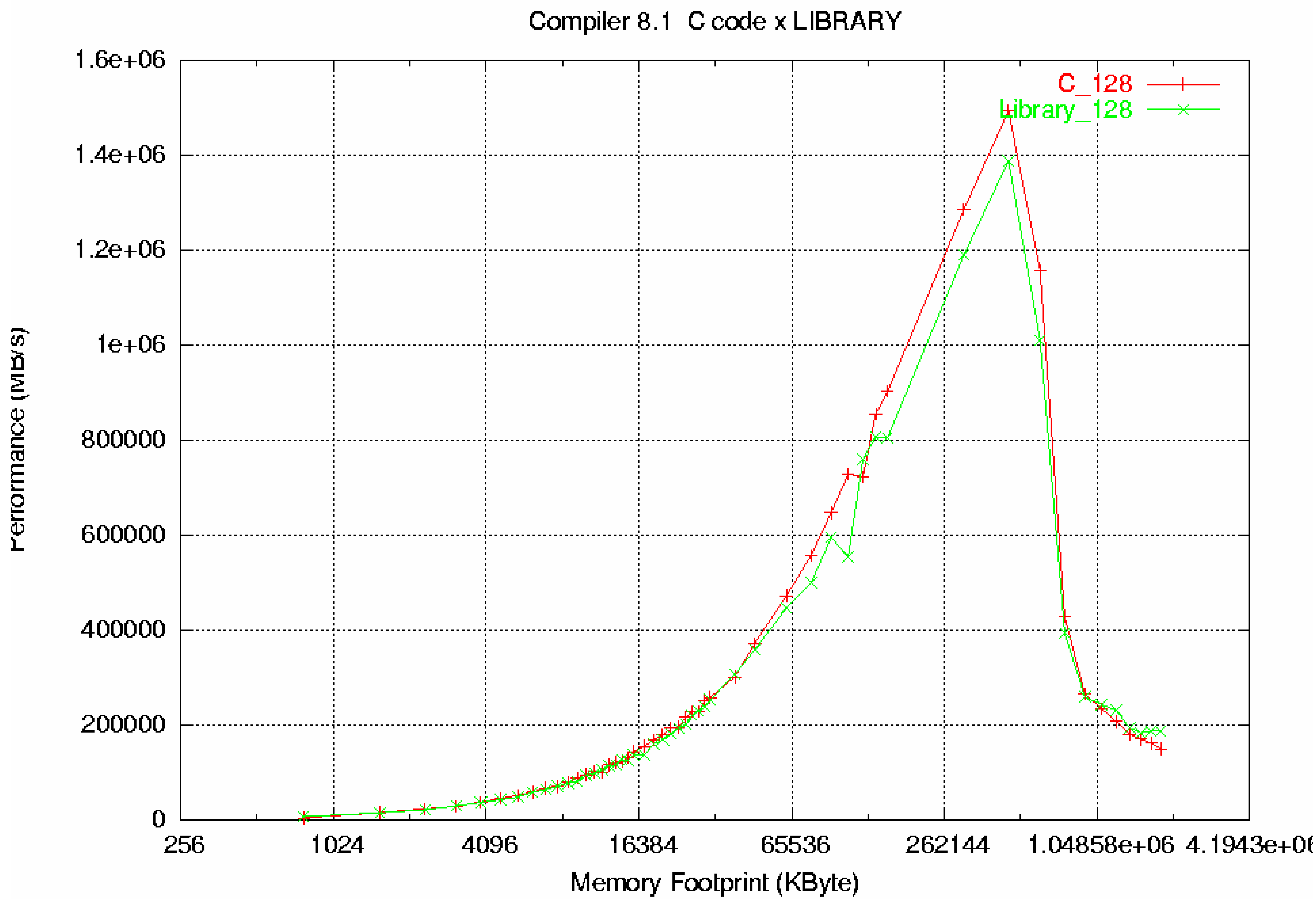

Compiler 8.0 C code x LIBRARY
C_128
Library_128
Performance (MB/s)
Memory Footprint (KByte)
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06

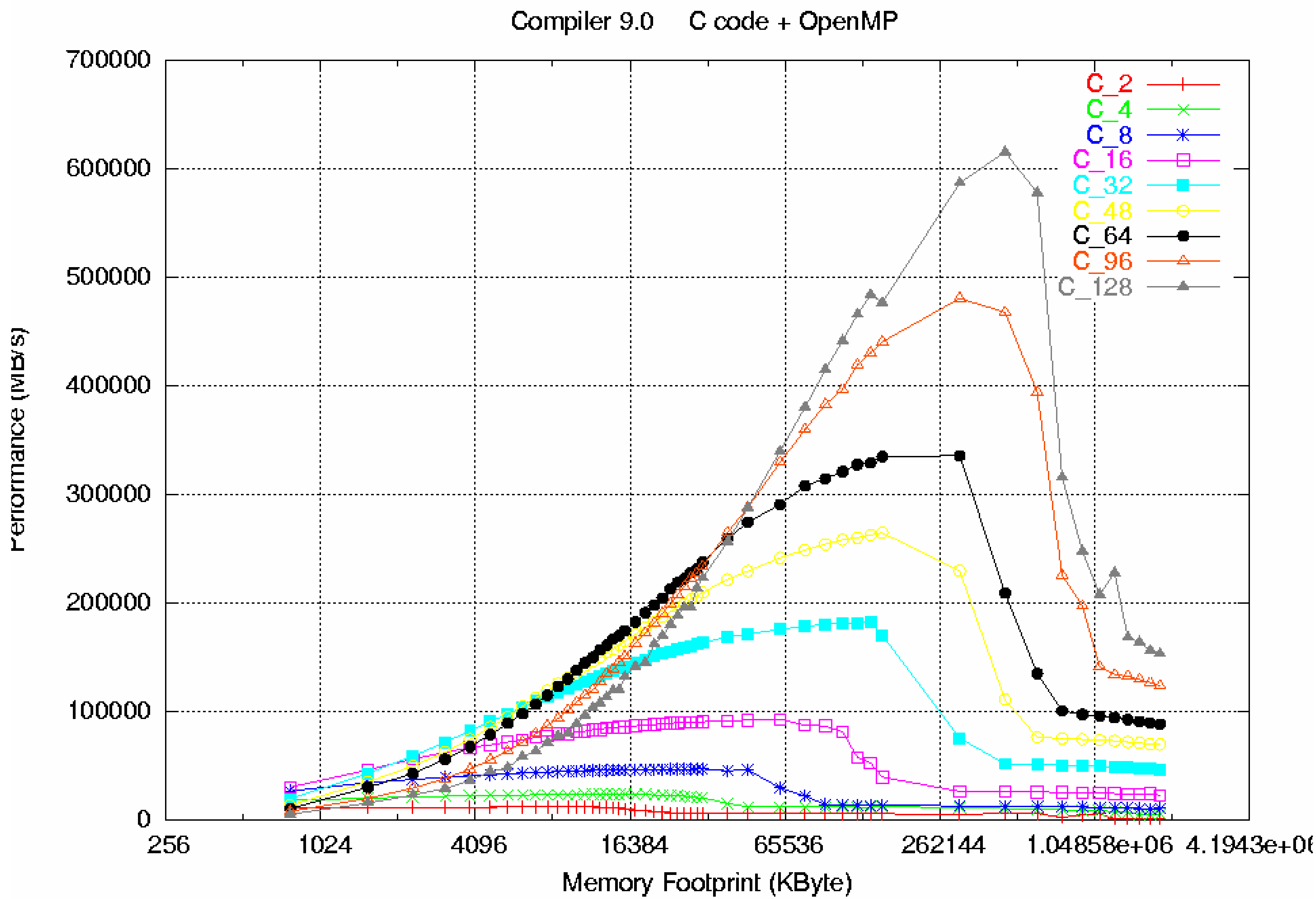

Compiler 8.1 C code + OpenMP
1.6e+06
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
Performance (MB/s)
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)
C_2
C_4
C_8
C_16
C_32
C_48
C_64
C_96
C_128


Compiler 8.1 dcopy from MKL + OpenMP
Performance (MB/s)
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
Memory Footprint (KByte)
Library_2
Library_4
Library_8
Library_16
Library_32
Library_48
Library_64
Library_96
Library_128

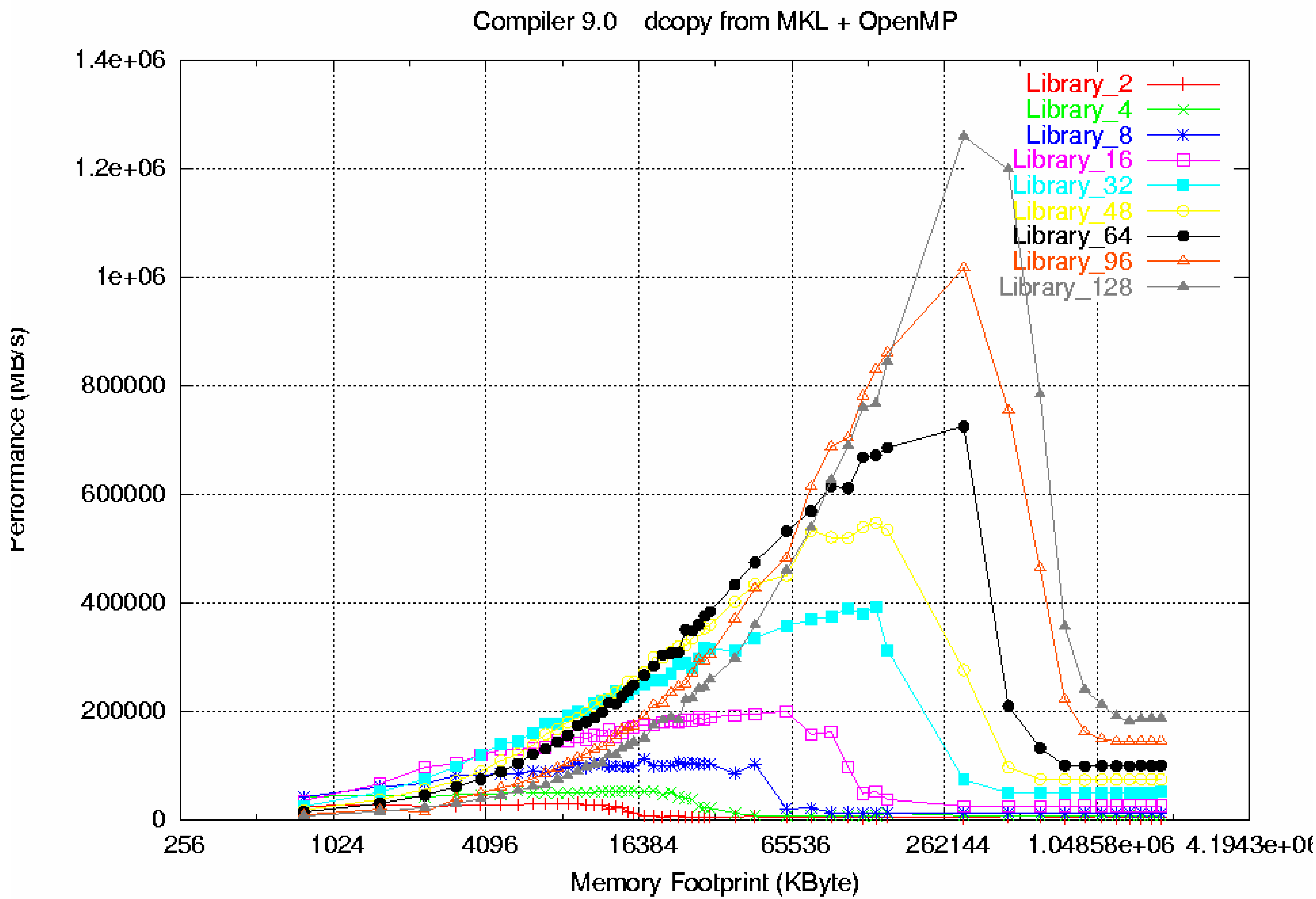


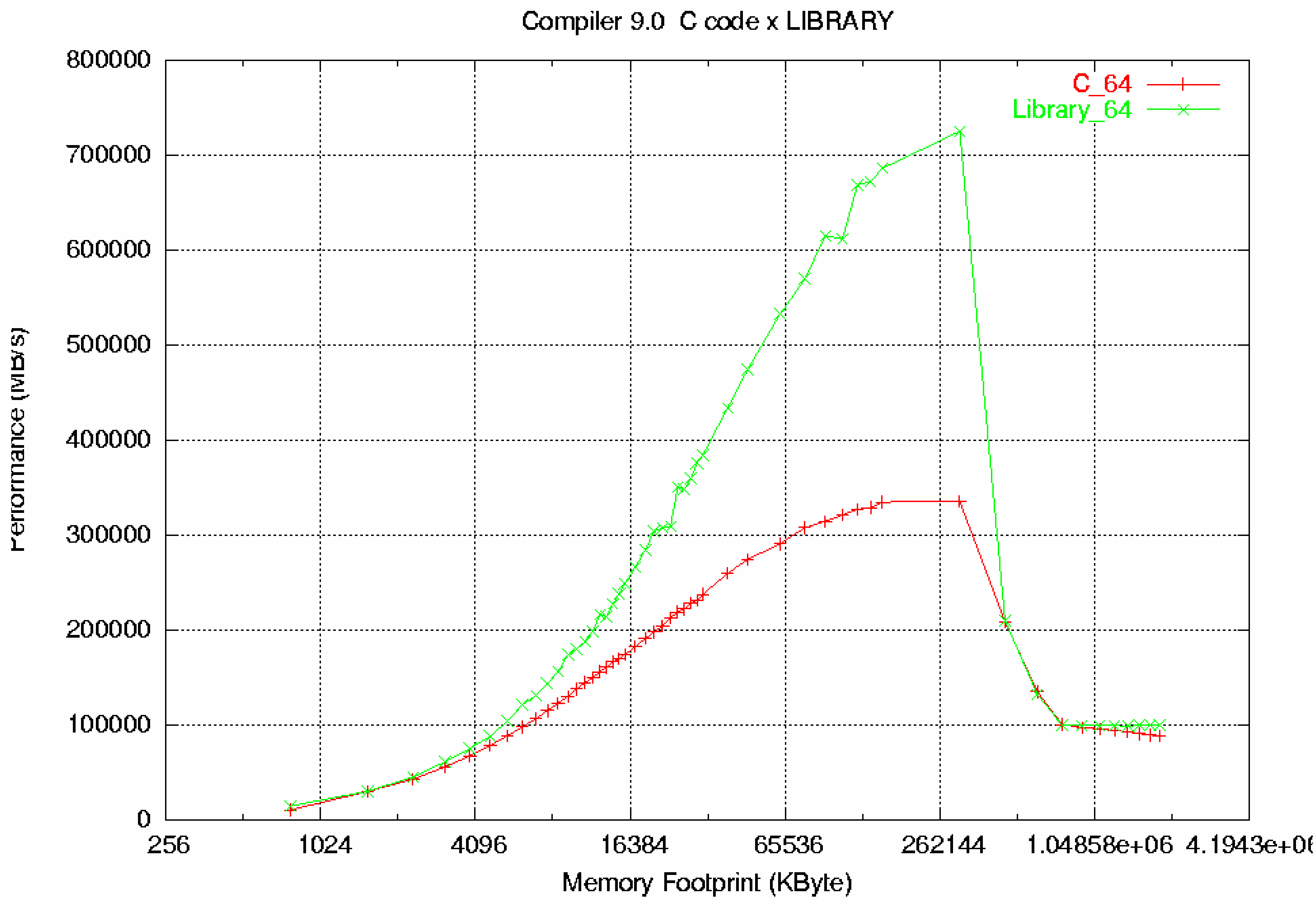
Compiler 8.1 C code x LIBRARY
C_64
Library_64
Performance (MB/s)
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)


Compiler 8.1 C code x LIBRARY
Performance (MB/s)
1.6e+06
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)
C_128
Library_128

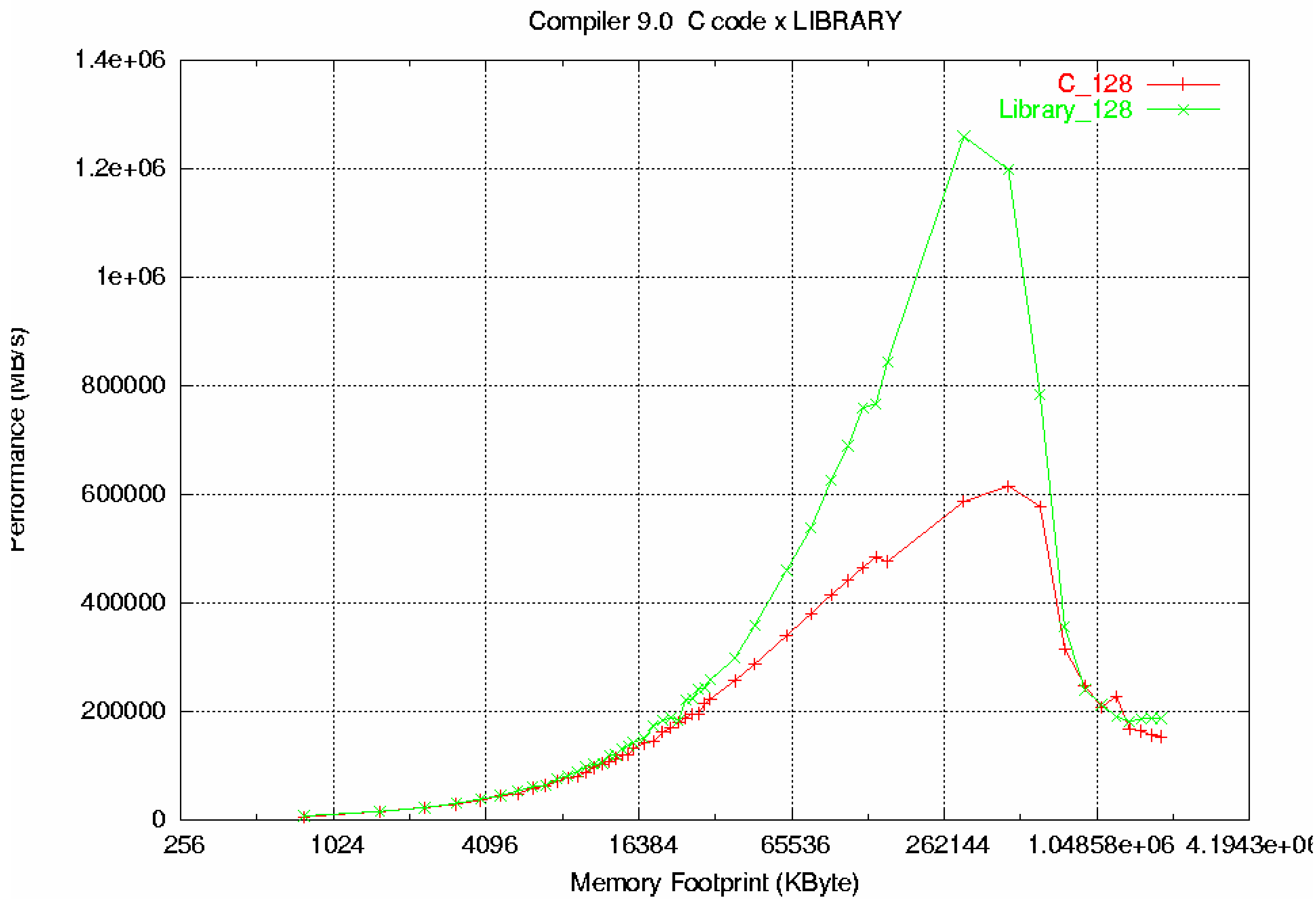


Compiler 9.0 C code + OpenMP
Performance (MB/s)
Memory Footprint (KByte)
700000
600000
500000
400000
300000
200000
100000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
C_2
C_4
C_8
C_16
C_32
C_48
C_64
C_96
C_128

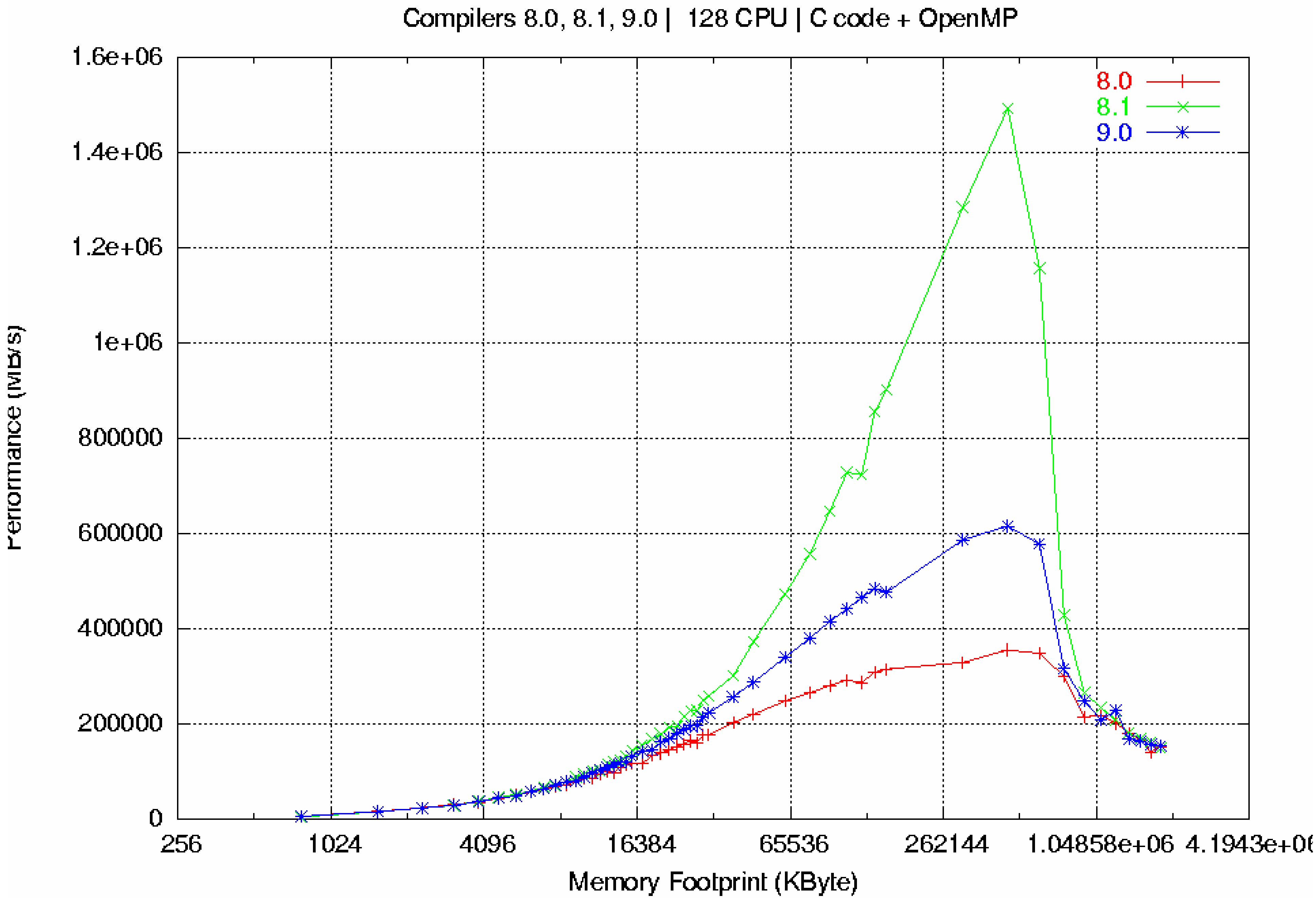

Compiler 9.0 dcopy from MKL + OpenMP
Performance (MB/s)
0
200000
400000
600000
800000
1e+06
1.2e+06
1.4e+06
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+0
Memory Footprint (KByte)
Library_2
Library_4
Library_8
Library_16
Library_32
Library_48
Library_64
Library_96
Library_128

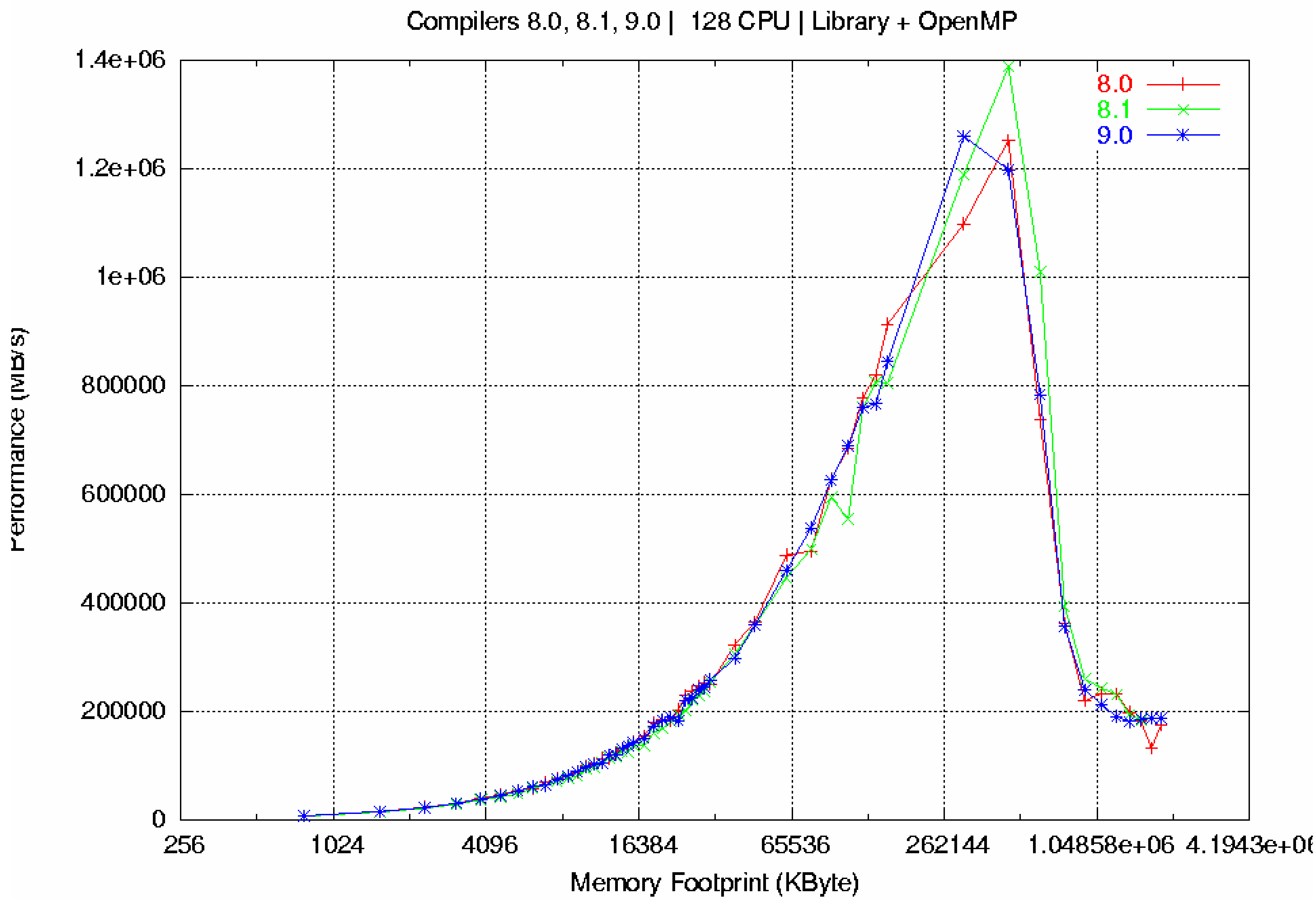


Compiler 9.0 C code x LIBRARY
C_64
Library_64
Performance (MB/s)
800000
700000
600000
500000
400000
300000
200000
100000
0
256
1024
4096
16384
65536
262144
1.04858e+06
Memory Footprint (KByte)



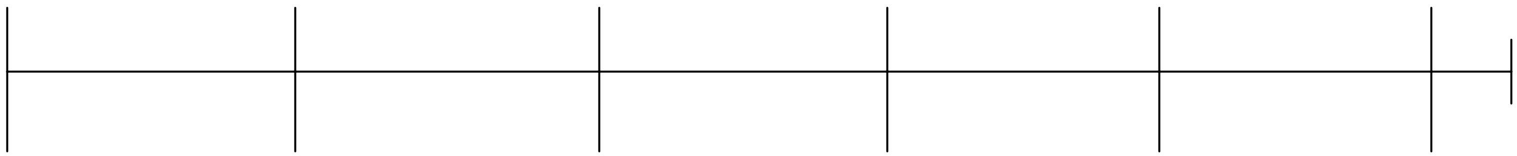
Compiler 9.0 C code x LIBRARY
C_128
Library_128
Performance (MB/s)
Memory Footprint (KByte)
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+0(


Compilers 8.0, 8.1, 9.0 | 128 CPU | C code + OpenMP
Performance (MB/s)
1.6e+06
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
Memory Footprint (KByte)
8.0
8.1
9.0



Compilers 8.0, 8.1, 9.0 | 128 CPU | Library + OpenMP
Performance (MB/s)
Memory Footprint (KByte)
8.0
8.1
9.0
1.4e+06
1.2e+06
1e+06
800000
600000
400000
200000
0
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06

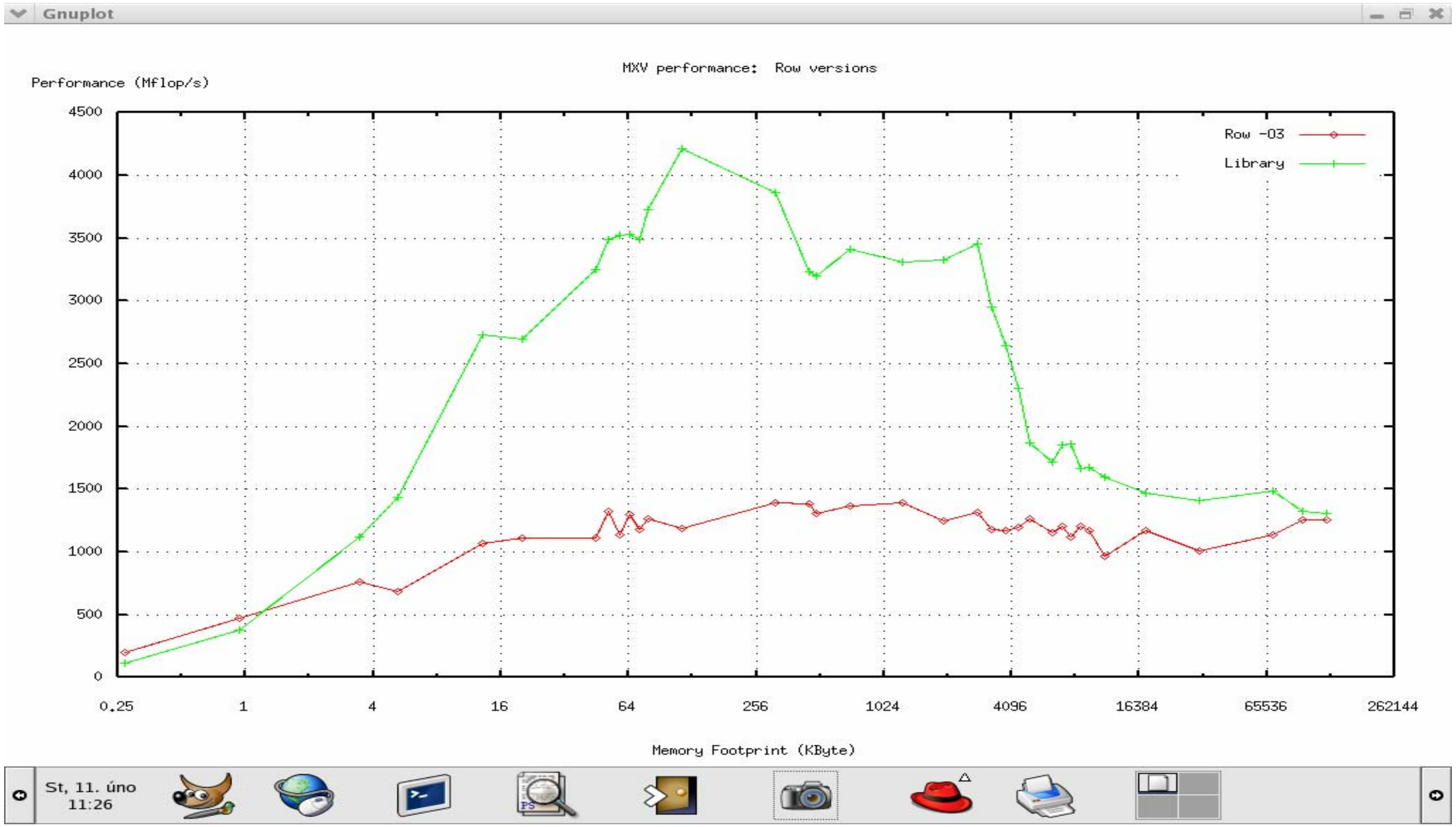
Library: cblas_dcopy(N,X,1,Y,1) & domain decomposition



```
#pragma omp parallel for
        for(i=0; i<nthreads; i++)
(void) cblas_dcopy(N/ nthreads, X + N/ nthreads * i, 1,
                              Y + N/ nthreads * i,1);
```

Matrix x vector

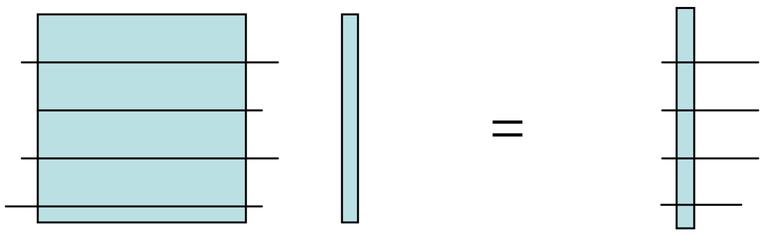
Serial function: dgemv (MKL, SCSL)



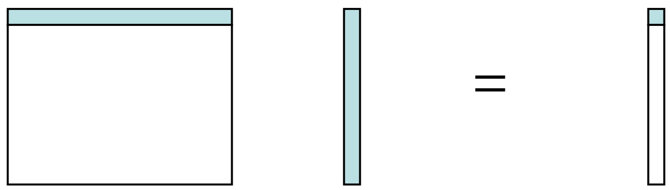
Parallel program   OpenMP   icc -openmp -O3

A) self-programmed C code

B) dgemv for rectangular submatrices

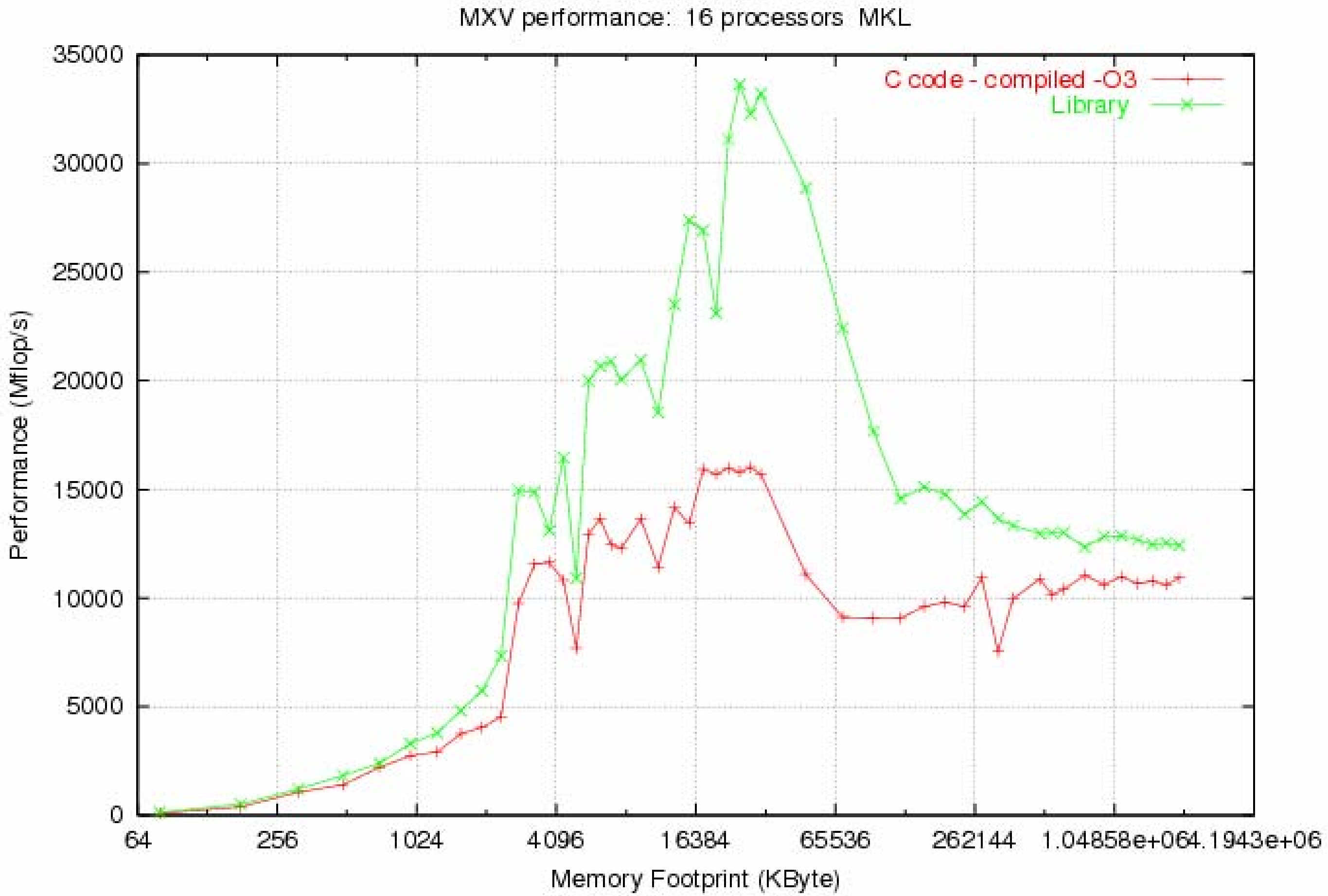


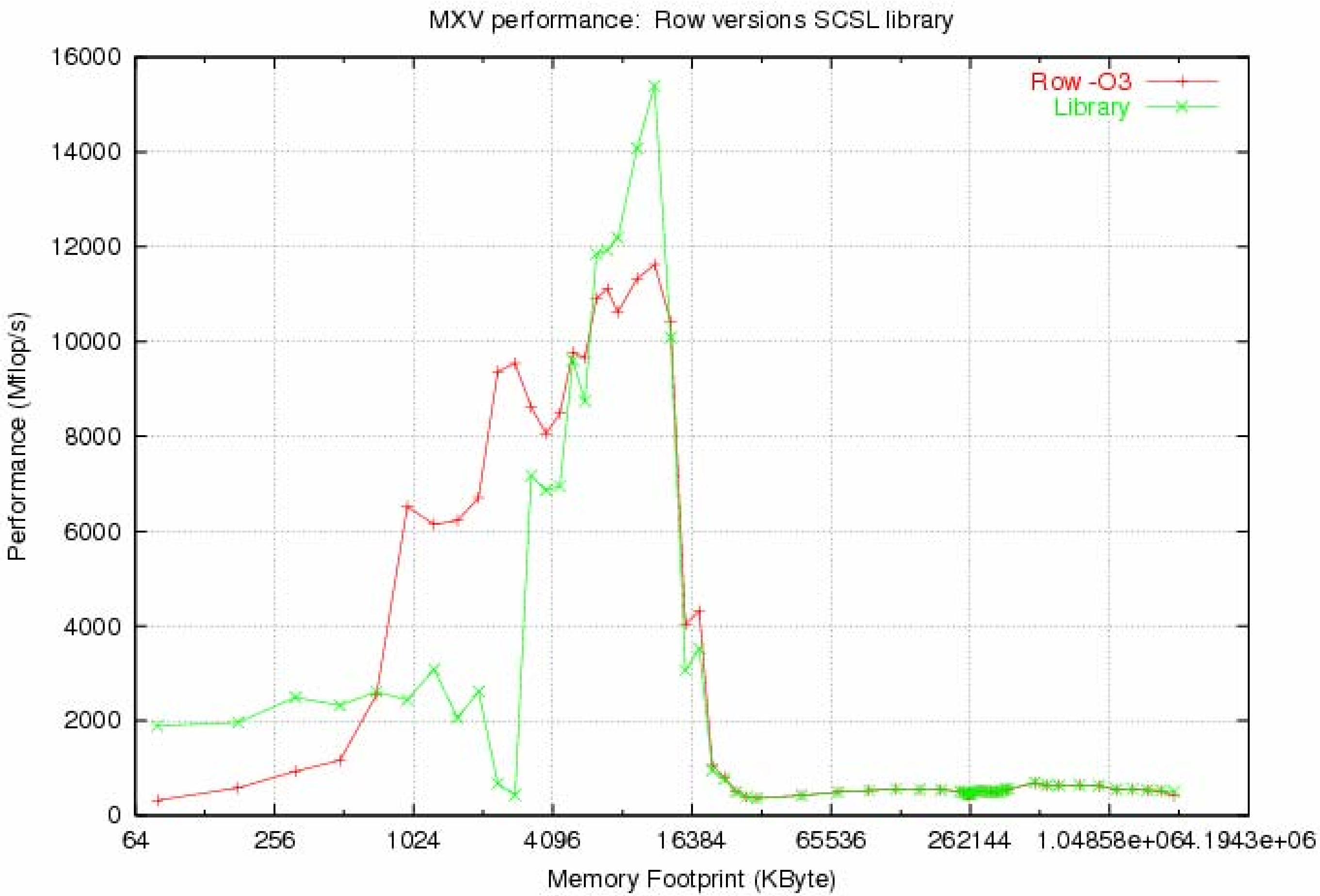
C) ddot function for scalar product of row and column



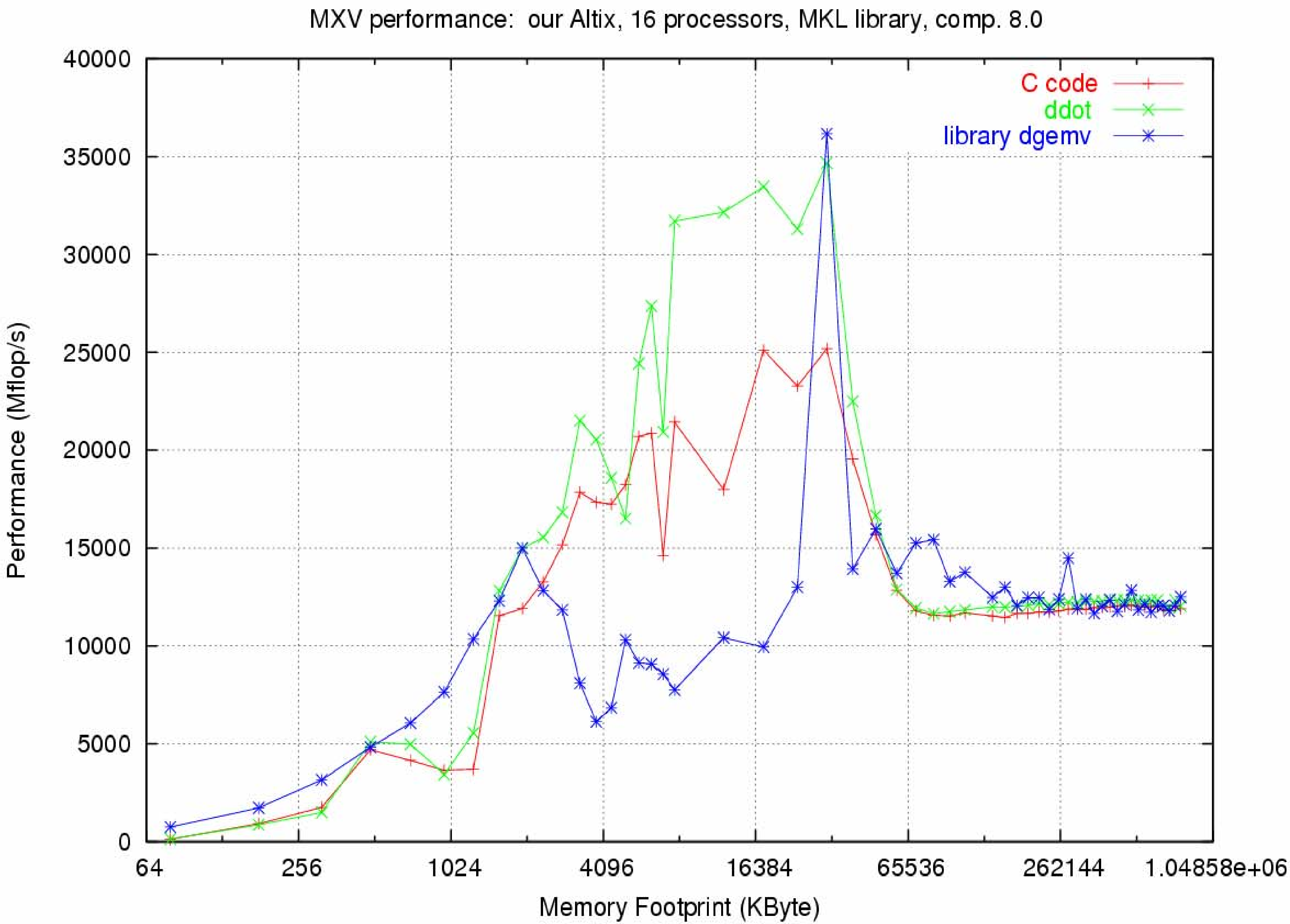
D) dgemv from SCSL (self-parallelizing)

Domain decomposition on „old“ hardware

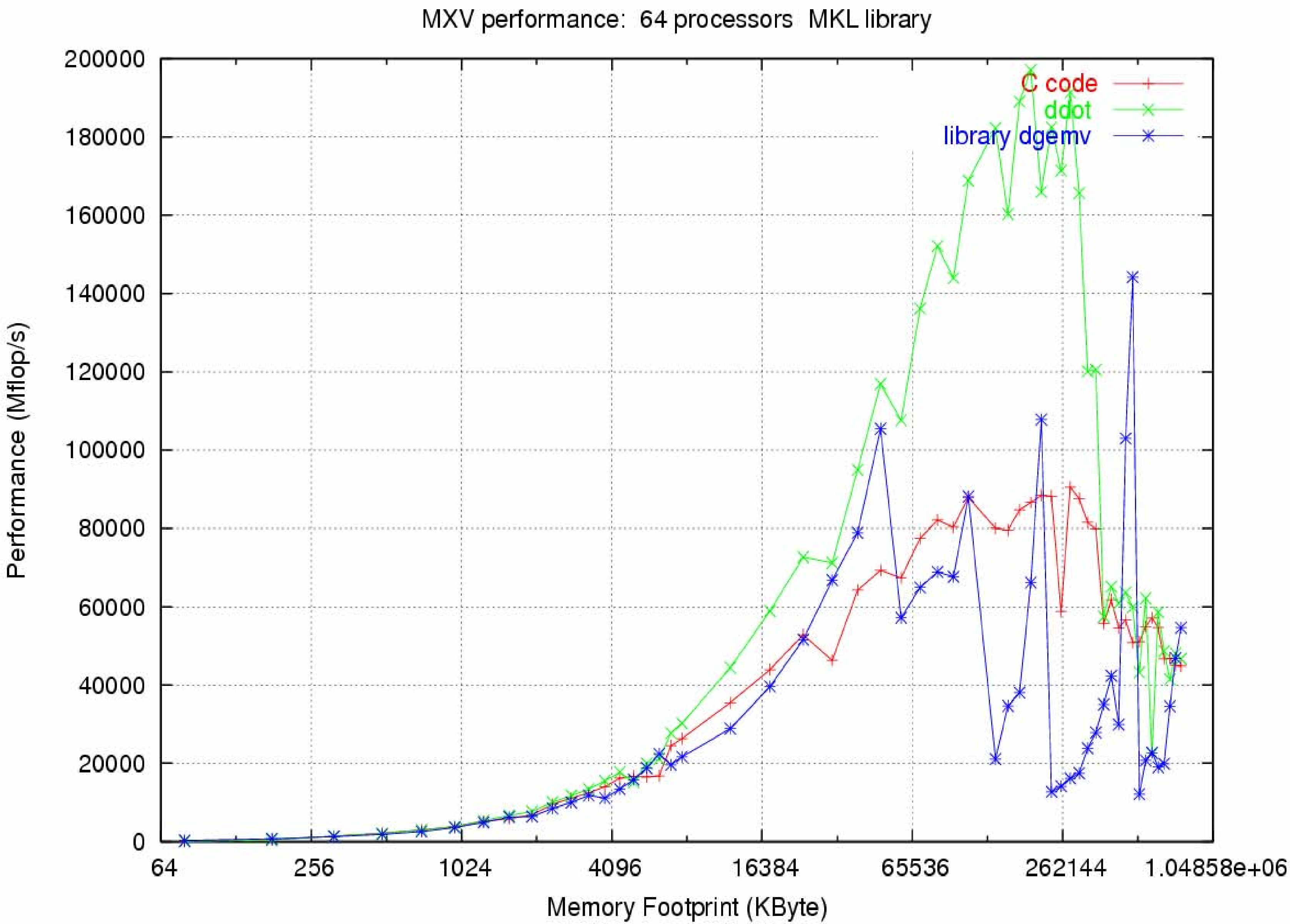




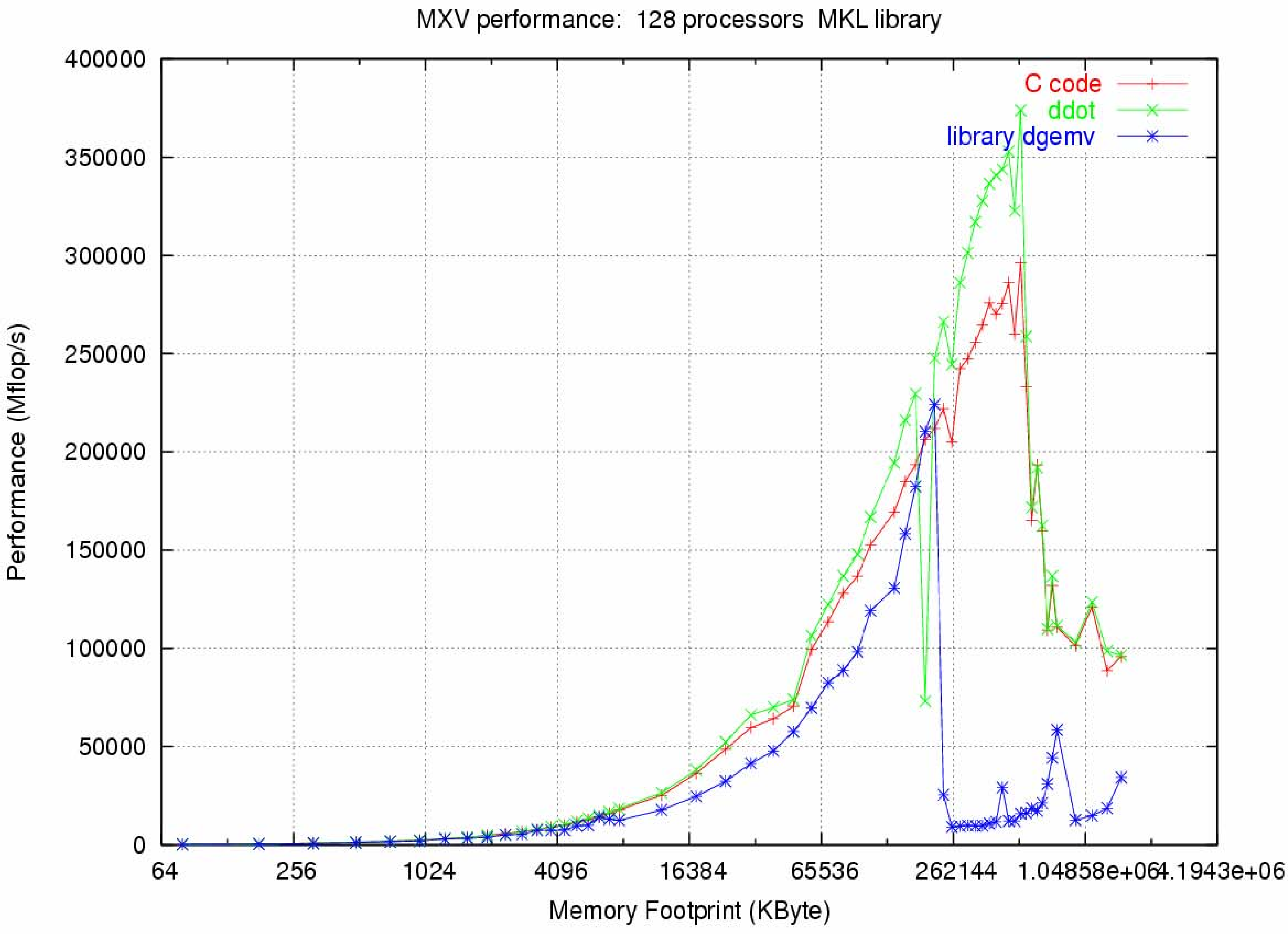
MXV performance: Row versions SCSL library
Row -O3
Library
Performance (Mflop/s)
Memory Footprint (KByte)
0
2000
4000
6000
8000
10000
12000
14000
16000
64
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06

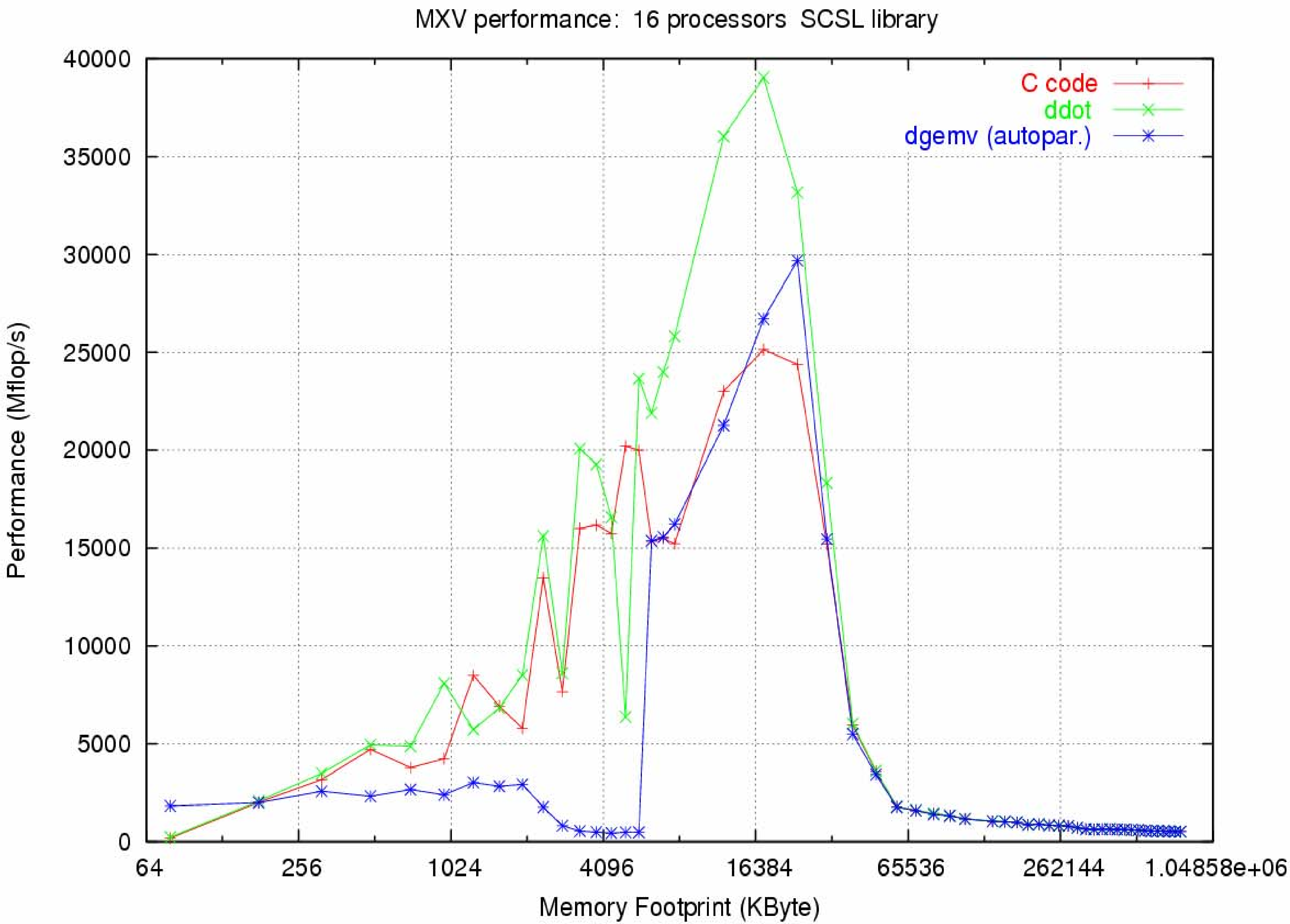


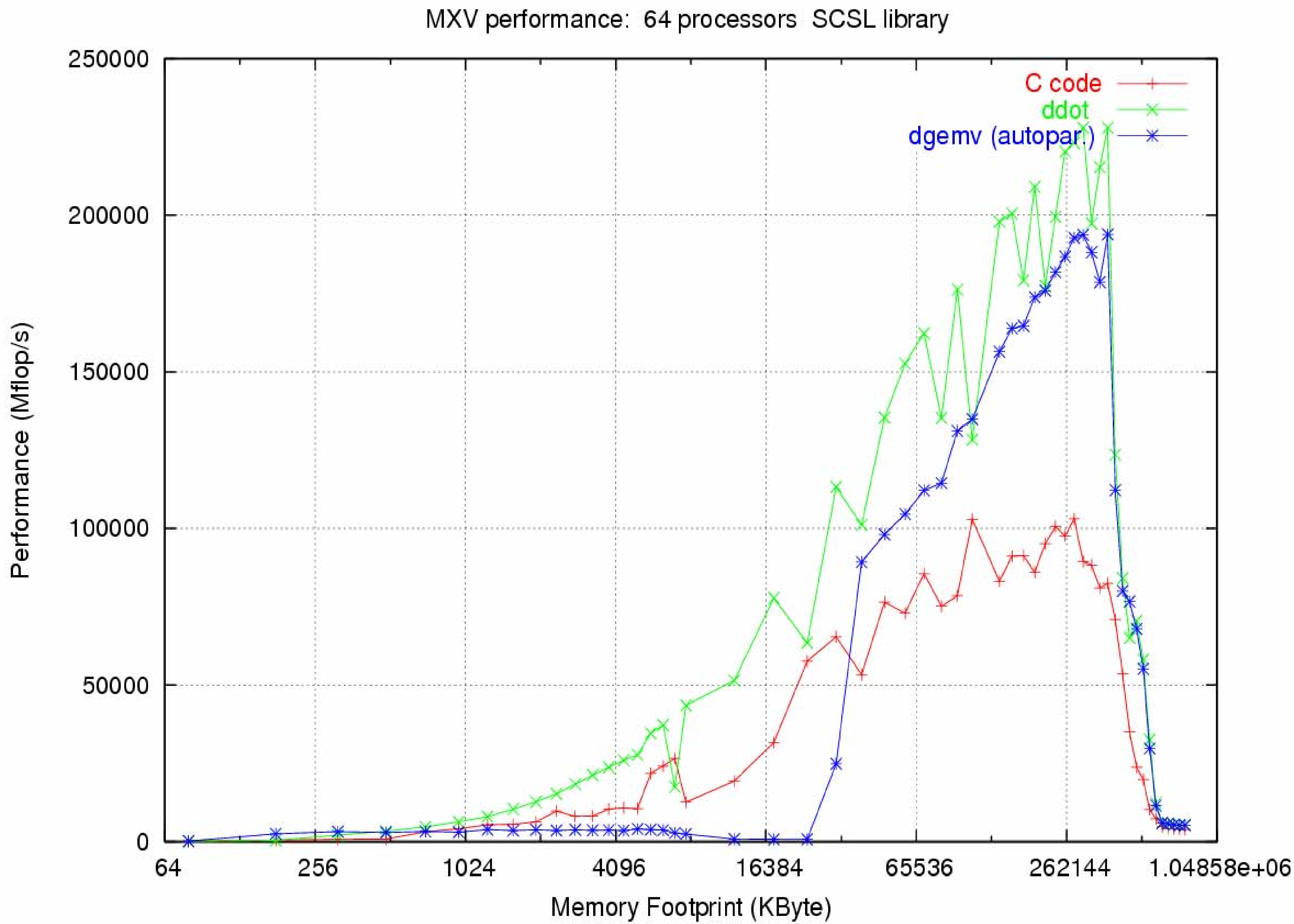
MXV performance: our Altix, 16 processors, MKL library, comp. 8.0
C code
ddot
library dgemv
Performance (Mflop/s)
0
5000
10000
15000
20000
25000
30000
35000
40000
64
256
1024
4096
16384
65536
262144
1.04858e+06
Memory Footprint (KByte)



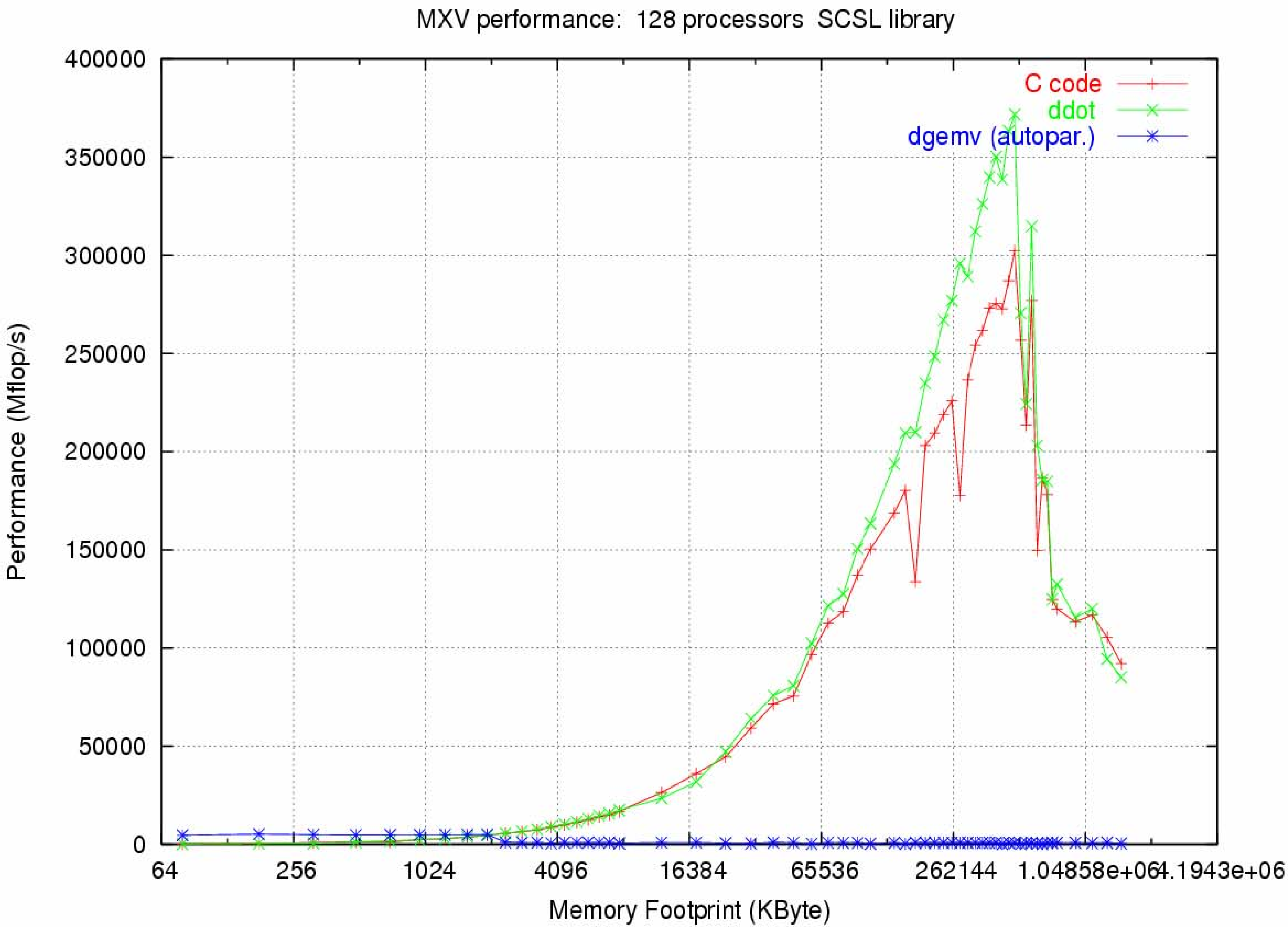
MXV performance: 64 processors MKL library
Performance (Mflop/s)
Memory Footprint (KByte)
C code
ddot
library dgemv
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
64
256
1024
4096
16384
65536
262144
1.04858e+06


MXV performance: 128 processors MKL library
C code
ddot
library dgemv
Performance (Mflop/s)
400000
350000
300000
250000
200000
150000
100000
50000
0
64
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)


MXV performance: 16 processors SCSL library
Performance (Mflop/s)
0
5000
10000
15000
20000
25000
30000
35000
40000
64
256
1024
4096
16384
65536
262144
1.04858e+06
Memory Footprint (KByte)
C code
ddot
dgemv (autopar.)



MXV performance: 64 processors SCSL library
C code
ddot
dgemv (autopar.)
Performance (Mflop/s)
0
50000
100000
150000
200000
250000
64
256
1024
4096
16384
65536
262144
1.04858e+06
Memory Footprint (KByte)


MXV performance: 128 processors SCSL library
C code
ddot
dgemv (autopar.)
Performance (Mflop/s)
400000
350000
300000
250000
200000
150000
100000
50000
0
64
256
1024
4096
16384
65536
262144
1.04858e+06
4.1943e+06
Memory Footprint (KByte)

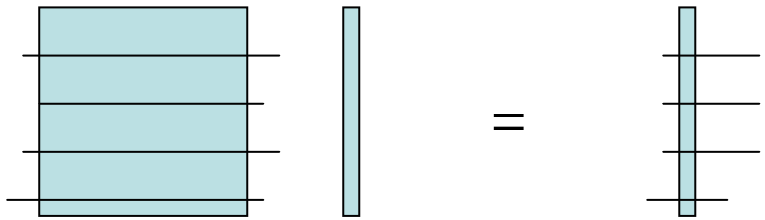
Parallel program

OpenMP

icc -openmp -O3

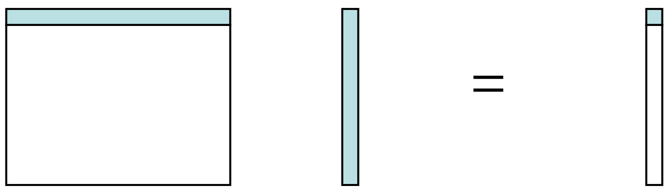
A) self-programmed C code

B) dgemv for rectangular submatrices



Altix 350

C) ddot function for scalar product of row and column



Altix 3700

D) dgemv from SCSL (self-parallelizing)

X

Contact:

pospisil@vc.cvut.cz