PGI® Compilers and Tools for AMD Opteron Processor-based CRAY Systems

Cray User Group Meeting
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STMicroelectronics
The Portland Group
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Outline

- CRAY/PGI Relationship
- PGI Compiler Architecture and Features
- Applications Porting/Tuning Resources
- PGI Compilers Basic Usage, Important Options
- Vectors are Back!
- Pending Tuning Issues, PGI Compilers Roadmap

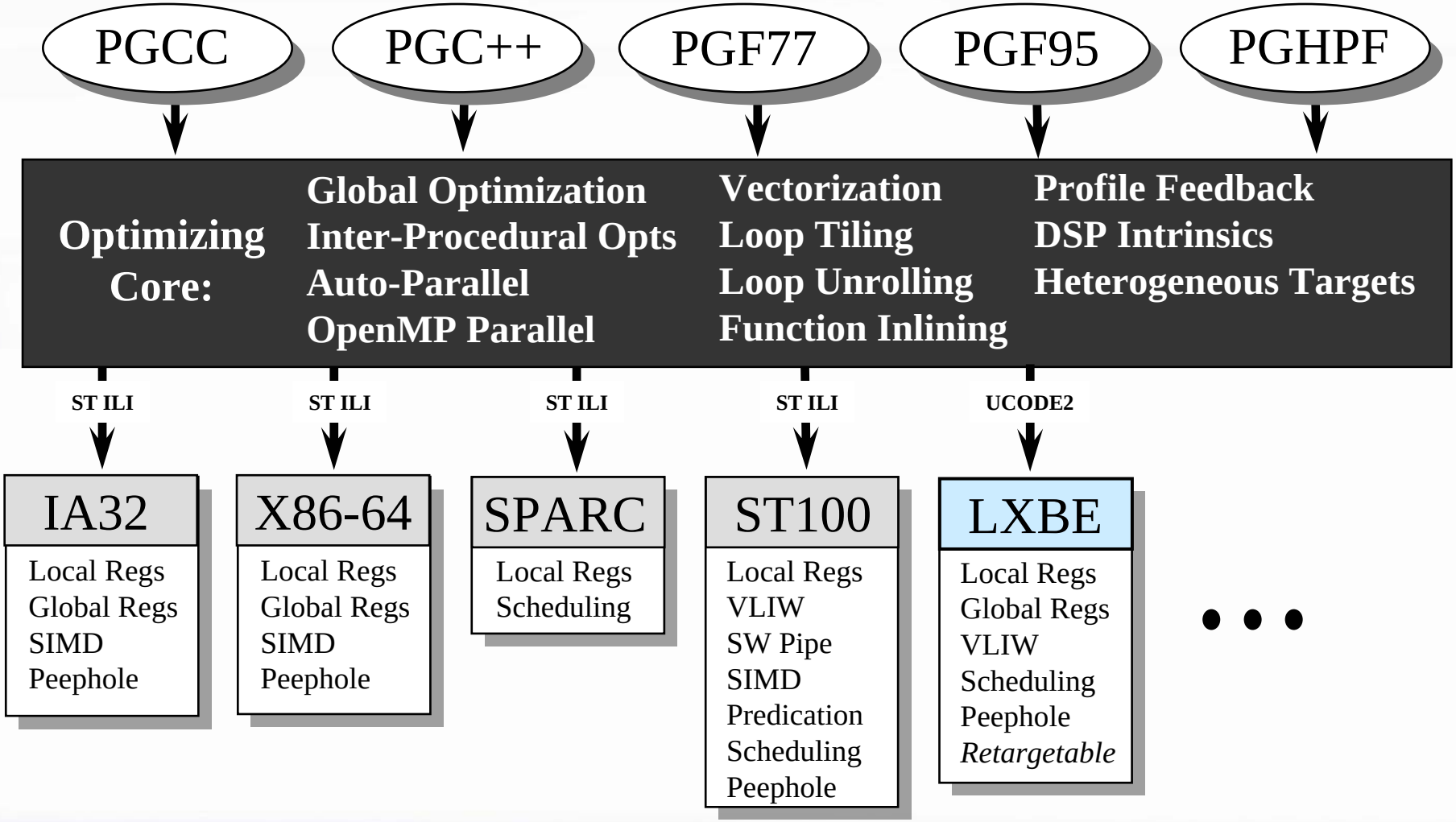
CRAY + PGI Relationship

- **CRAY/PGI History** – PGHPF/CRAFT for CRAY T3E (1996)
- **PGI ASCI History** – ASCI Red F90/C/C++ for Sandia (1997)
- **PGI on Linux86** – Production F90/C/C++ compilers (1997)
- **PGI on AMD Opteron** – Cooperation with AMD (2002)
- **ASCI + CRAY + Opteron Red Storm** ➔ CRAY + PGI
- **CRAY/PGI Agreement** – CRAY resells and supports PGI F95/C/C++ on Red Storm, CRAY XT3, CRAY XD1 (2004)

Who Does What?

- **Development** – Compiler development/QA by PGI
- **CRAY Integration** – Add'l CRAY testing and integration on target HW and OS
- **Applications, Benchmarking** – Both
- **Technical Support** – Frontline support by CRAY, compiler bugs to PGI for fixing and (if needed) help finding bug workarounds
- **Release Schedules** – Standard PGI release schedules; usually 2 per year (one major, one minor) and several "builds" of each release for tech support / new OSs / etc; current release is **6.0-4**

PGI Compilers



PGI Compilers Key Features

- **Optimization** – State-of-the-art optimization infrastructure
- **Cross-platform** – AMD & Intel, 32- & 64-bit, Linux & Windows
- **Tools** – F95/C/C++ debugger/profiler, doc's, pgroup.com
- **Comprehensive Linux Support** – Red Hat 7.3 – 9.0, RHEL 3.0/4.0, Fedora Core 2/3, SuSE 7.1 – 9.2, SLES 8/9
- **Parallel** – OpenMP/MPI supported in all languages and tools
- **Infrastructure** – NAG, VNI, ACML, TotalView, ISV App's, Research App's, Research Tools, PAPI

Commercial Applications Porting to 64-bit x86 with PGI Compilers

- **MCAE** – ANSYS*, ADINA*, MSC.MARC*, NX NASTRAN
- **Computational Chemistry** – GAUSSIAN*
- **Automotive** – LS-DYNA*, PAM-CRASH, PAM-STAMP, RADIOSS*, MADYMO
- **CFD** – STAR-CD*, Fluent POLYFLOW*, AVL Fire*
- **Geophysical** – Several Proprietary
- **Math Libraries** – ACML*, NAG*

*In production

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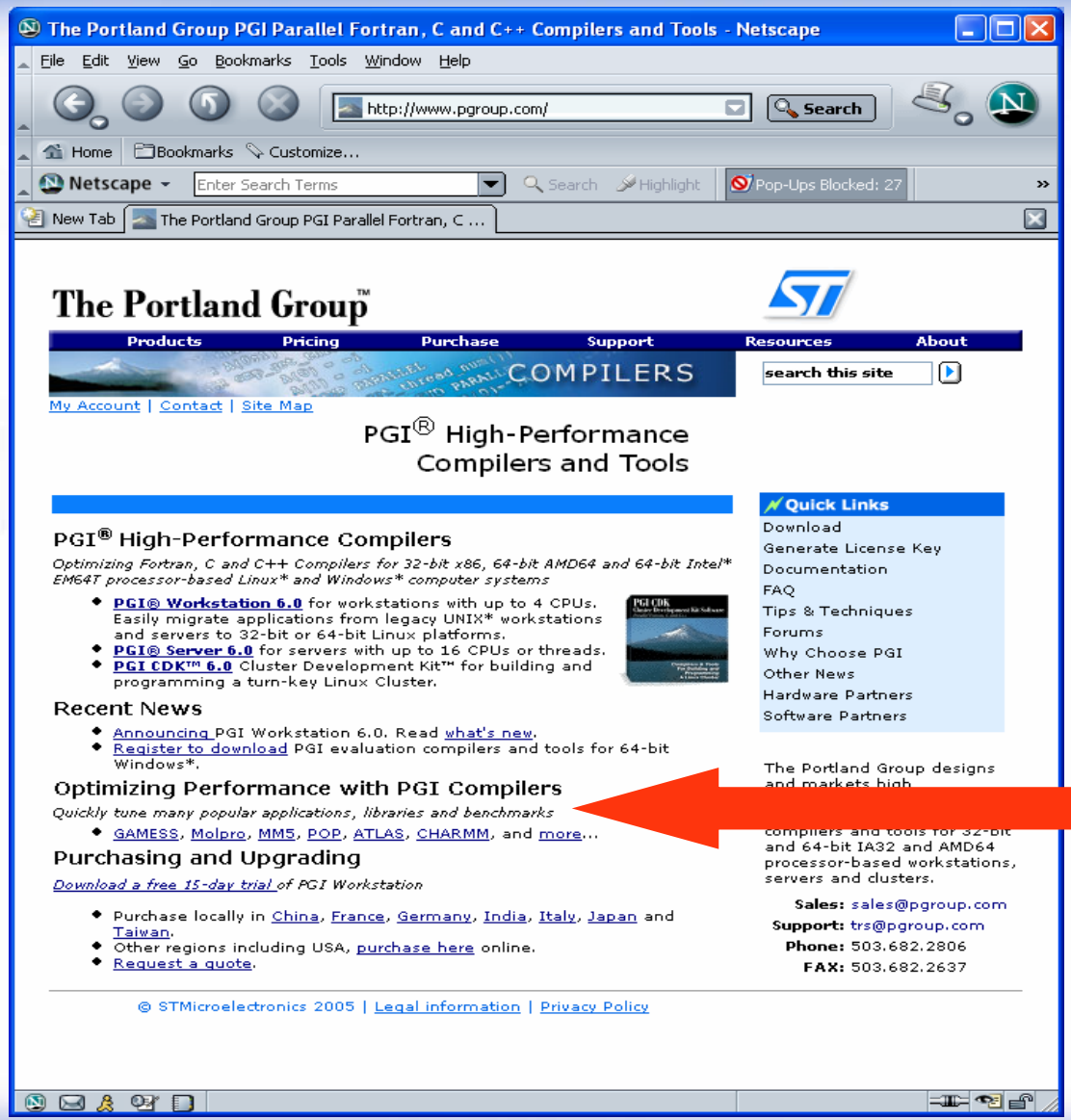
Research Applications Pre-tested with PGI Compilers

- **Weather** – MM5, WRF2, POP, MOM4, CAM
- **Computational Chemistry** – GAMESS, AMBER, MOLPRO, CHARMM, PWSCF
- **Bioinformatics** – BLAST
- **DOE/DOD** – MCNP5, TBMD
- **Libraries** – ATLAS, OPENGL, NetCDF, MPICH, MPICH-GM



pgroup.com

- License/Seat Mgmt
- Documentation
- Online FAQs
- Online User Forums
- Extensive App's porting and tuning guides

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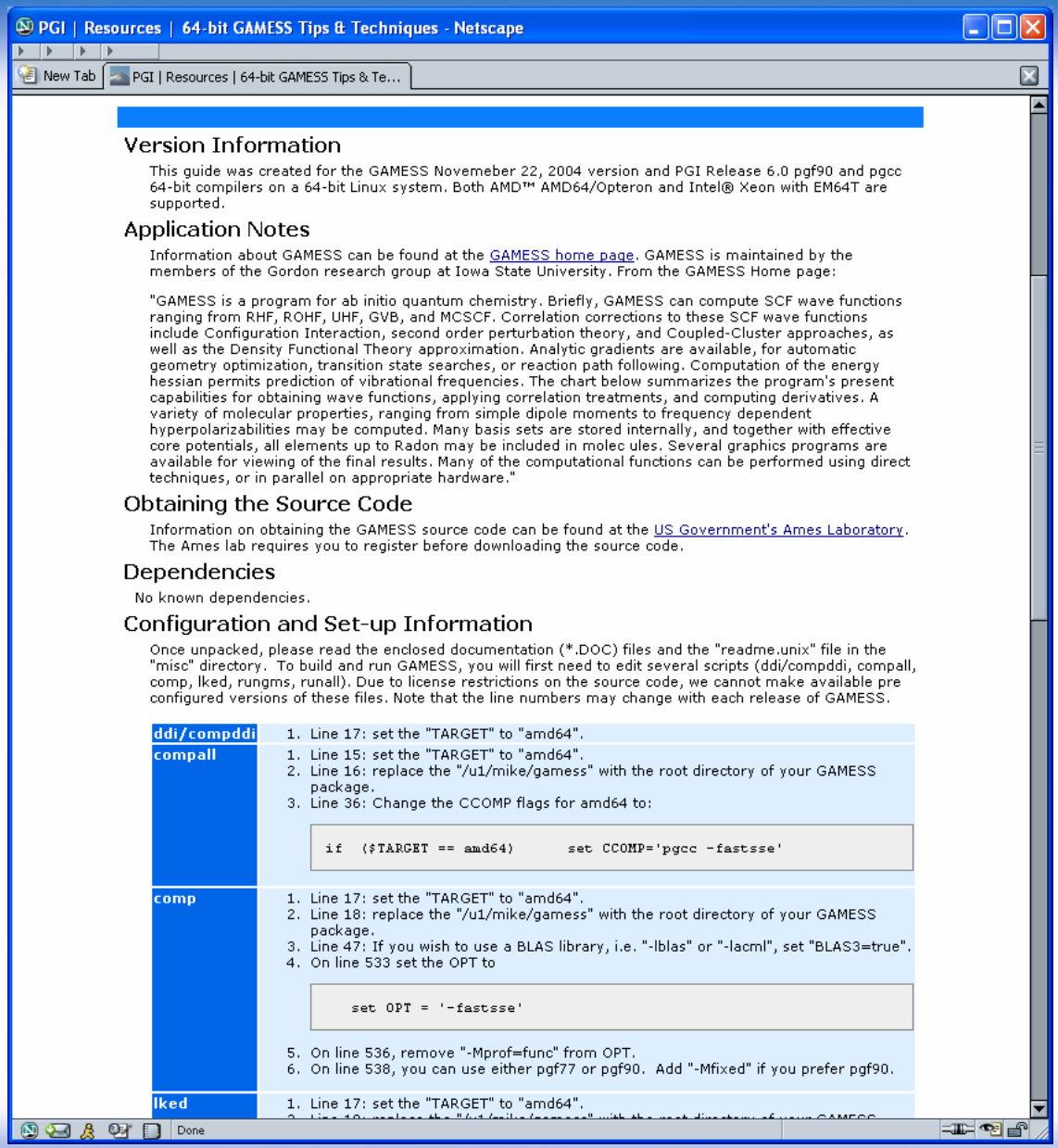

GAMESS Application Note on pgroup.com

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Basic Usage of PGI Compilers

- **Compiler *drivers*** – interpret options and invoke pre-processing, compilers, IPA, assembler, linker
- **Options precedence** – if two or more options conflict, last option on command line takes precedence
- **Use `-help`** – to list all options or see details on how to use a given option, e.g. **`pgf95 -fastsse -help`**
- **Use `-Minfo`** – to see a compile-time listing of optimizations and transformations performed by the compiler
- **PGI User's Guide** – chapters 2 and 3 – 35 pages that will make you an expert at using the PGI compilers

Important PGI Compiler Options

-fast	Includes "`-O2 -Munroll –Mnoframe -Mlre`"
-fastsse	Includes "`-fast –Mvect=sse -Mcache_align`"
-Mipa=fast	Enable inter-procedural analysis (IPA) and optimization
-Mipa=fast,inline	Enable IPA-based optimization *and* function inlining
-Mpfi … -Mpfo	Enable profile- and data-feedback based optimizations
-Minline	Inline functions and subroutines
-Mconcur	Try to auto-parallelize loops for SMP/Dual-core systems
-mp[=align]	Process OpenMP/SGI directives and pragmas
-mcmodel=medium	Enable data > 2GB on AMD64/EM64T running 64-bit Linux
-Minfo	Compile-time optimization/parallelization messages
-help	Compiler options and usage

`–fastsse –Mipa=fast` usually best for "compile-and-go"

Vectorizable Loop in SPECFP2K FACEREC Data is REAL*4

```
350 !
351 !   Initialize vertex, similarity and coordinate arrays
352 !
353     Do Index = 1, NodeCount
354       IX = MOD (Index - 1, NodesX) + 1
355       IY = ((Index - 1) / NodesX) + 1
356       CoordX (IX, IY) = Position (1) + (IX - 1) * StepX
357       CoordY (IX, IY) = Position (2) + (IY - 1) * StepY
358       JetSim (Index)  = SUM (Graph (:, :, Index) * &
359     &                   GaborTrafo (:, :, CoordX(IX,IY), CoordY(IX,IY)))
360       VertexX (Index) = MOD (Params%Graph%RandomIndex (Index) - 1, NodesX) + 1
361       VertexY (Index) = ((Params%Graph%RandomIndex (Index) - 1) / NodesX) + 1
362     End Do
```

Inner loop at line 358 is vectorizable, can used packed SSE instructions

Use –Minfo to see Which Loops Vectorize

```
% pgf95 -fastsse -Mipa=fast -Minfo -S graphRoutines.f90
…
localmove:
   334, Loop unrolled 1 times (completely unrolled)
   343, Loop unrolled 2 times (completely unrolled)
   358, Generating vector sse code for inner loop
   364, Generating vector sse code for inner loop
        Generating vector sse code for inner loop
   392, Generating vector sse code for inner loop
   423, Generating vector sse code for inner loop
%
```

Scalar SSE:

```
.LB6_668:
# lineno: 358
        movss   -12(%eax),%xmm1
        movss   -8(%eax),%xmm2
        movss   -4(%eax),%xmm3
        decl    %edx
        mulss   -12(%ecx),%xmm1
        addss   -572(%ebp),%xmm1
        mulss   -8(%ecx),%xmm2
        addss   %xmm2,%xmm1
        mulss   -4(%ecx),%xmm3
        addss   %xmm3,%xmm1
        movss   (%eax),%xmm2
        addl    $16,%eax
        mulss   (%ecx),%xmm2
        addl    $16,%ecx
        addss   %xmm2,%xmm1
        testl   %edx,%edx
        movss   %xmm1,-572(%ebp)
        jg      .LB6_668
```

Vector SSE:

```
.LB6_1105:
# lineno: 358
        movlps  (%esi,%ecx),%xmm2
        movlps  (%edx,%ecx),%xmm3
        movhps  8(%esi,%ecx),%xmm2
        movhps  8(%edx,%ecx),%xmm3
        mulps   %xmm2,%xmm3
        movlps  16(%esi,%ecx),%xmm2
        movhps  24(%esi,%ecx),%xmm2
        addps   %xmm3,%xmm0
        movlps  16(%edx,%ecx),%xmm3
        movhps  24(%edx,%ecx),%xmm3
        addl    $32,%ecx
        mulps   %xmm2,%xmm3
        addps   %xmm3,%xmm0
        subl    $8,%eax
        jg      .LB6_1105
```

Facerec Scalar: 104.2 sec
Facerec Vector: 84.3 sec

Maximizing Vectorization

- May need to split “large” loops by hand (or try –Mvect=nosizelimit)
- Don’t unroll loops by hand – re-roll if necessary to enable vectorization and let the compiler unroll loops where needed (or use –Munroll)
- Fortran 90 POINTER may not be contiguous
- Index arrays can prevent vectorization, or make it inefficient
- Check asm code to see if `movaps` / `movapd` used
- Vectorization is not always profitable, especially double-precision
- Double-precision scalar vs vector peak speed is the same, but vectorized loops have fewer instructions, can use aligned moves

Pending Compiler Tuning Issues

- **C/C++ Inlining** – funcs returning struct, funcs w/statics, alloca, operators
- **C/C++ General** – global optz across non-loop blocks, scalar replacement of aggregates, better idiom recognition, mitigating load after store penalties (primarily for EM64T), eliminate useless struct copies
- **C++** – re-implement trap handler / --no_exceptions, EDG IL optz
- **OpenMP PARALLEL DO iterations** – alignment versus load balancing
- **OpenMP thread CPU hopping** – sched_setaffinity() a little flakey
- **NUMA on AMD Opteron** – ensure memory is node-local, need NUMA-aware OpenMP runtime library
- **Autoparallel on Dual-core** – How effective can we make it?
- **Prefetching** – non-vector loops, prefetching for indirect, directives
- **EM64T-specific Issues** – seem to be a lot of them; characterizing

PGI Compilers & Tools Roadmap

- **PGI 6.0-5 in June, PGI 6.1 in November**
- **More Performance Tuning**
  - C/C++ tuning – IPA, inlining, pointer opt's, EDG IL opt's, etc (6.1)
  - Dual-core – Support/Tuning/OpenMP (6.0-5, more in 6.1)
  - OpenMP – DYNAMIC, GUIDED, runtime efficiency (6.0-5), NUMA (6.1)
  - AMD64, IA32, EM64T code generator tuning (6.1)
  - F95 optimizations (6.1 – need examples of object-oriented F95!)
  - Vectorizer – splitting, partial vect, transcendentals, conditionals, etc (6.1)
  - Track/tune more end-user & ISV applications (ongoing)
  - Hand-coded math libs (6.1)
- **Language/Compiler Features** – C99, OpenMP 2.5, SSE3, GNU asm (6.1)
- **Tools Features** – PGI Visual Fortran; VS05 integration on Win64
- **Documentation** – Can we simplify?
- **Operating Systems** – SuSE, Red Hat, 64-bit Windows

Questions?