IBM Research GmbH Zurich Research Laboratory

Extending the scalability of electronic structure calculations by algorithms re-engineering

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IBM

Outline of the Presentation

- Introduction
  - Computational Sciences at IBM Zurich Research Laboratory
  - The need of extreme parallelism
- The CPMD code: a research tool for ab-initio MD
  - CPMD parallelization and scaleout
  - Cache/Network Optimized Orthogonalization
  - Performance on tests systems : time scales and system sizes
- The new challenges toward exascale computing
  - Fault tolerant and energy efficient algorithms
- Succesfull application examples
- Conclusions

IBM Research - Zurich

Since 1956

40 different nationalities

90 Collaborative projects with universities, industrial partners and governments

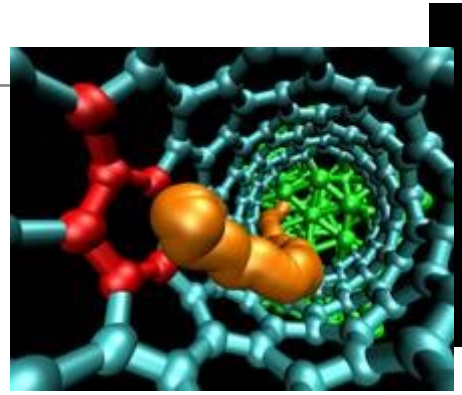
Two Nobel Prizes (1986 and 1987)

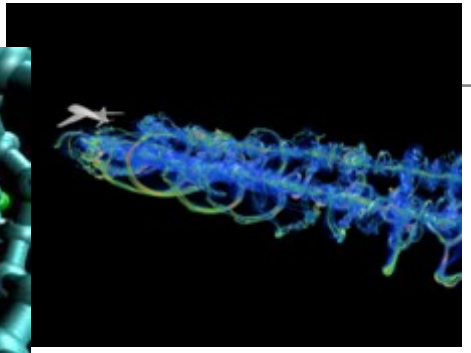
New Nanotech Center opened in 2011

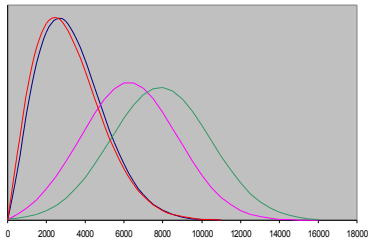
Mathematical & Computational Science

Business Optimization

- Inventory Optimization
- Optimization under uncertainty





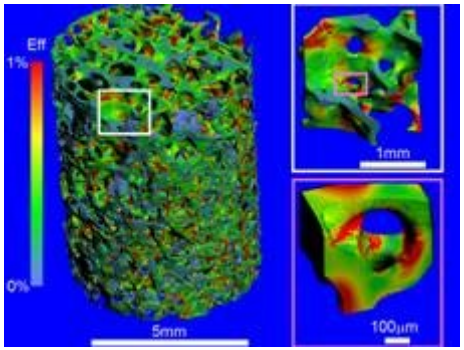


Computational Sciences

- Simulation of complex systems
- Supercomputing applications

Data Analytics

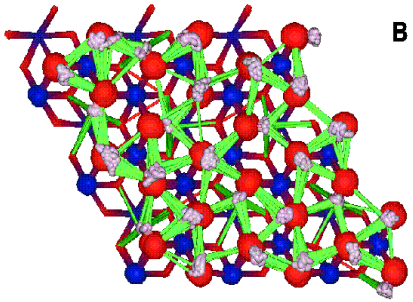
- Operational Risk
- Customer analytics



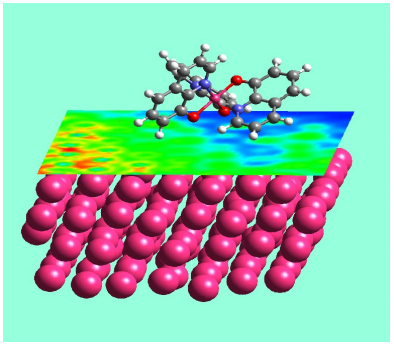
Computational Science at ZRL

- Developing and applying atomistic simulation techniques
  - Ab-initio Molecular Dynamics
  - Large Scale Classical Molecular Dynamics
  - Reactive Force Fields optimization and design
  - Multiscales simulations
- Applications to relevant IBM technology problems such as:
  - High-K materials
  - Defects diffusion in Si/SiO2 systems
  - Metal-CNTs contacts
  - Strain dependent transport properties of Si nanowires
  - Nano-Molecular switches
- Applications to relevant problems of key industries:
  - Enzymatic Reactions and Drug design
  - Accurate materials simulations (e.g. materials aging)
  - Energy production and Energy Storage
  - Micro – Finite Elements simulations
  - DNS Computational Fluid Dynamics
- Algorithm development and scaleout for simulation of complex systems
- Collaborations and Joint Projects with key partners such as:
  - ABB, Egypt government, Novozymes, Nestle Research, Ford Research, Mitsubishi Chemical, Akzo Nobel, Merck, Novartis,…

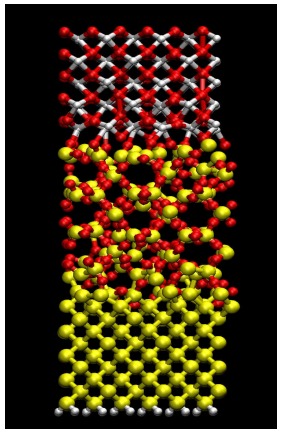
Real Examples



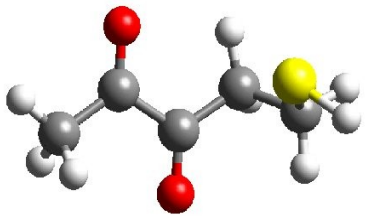
- Corrosion of Aluminum by Water
  - with Ford Research
    Science 282, 265 (1998)



- Materials for OLED or Organic Electronics
  - Applied Physics Letters 80, 2517 (2002)
  - Physical Review Letters 98, 076803(2007)

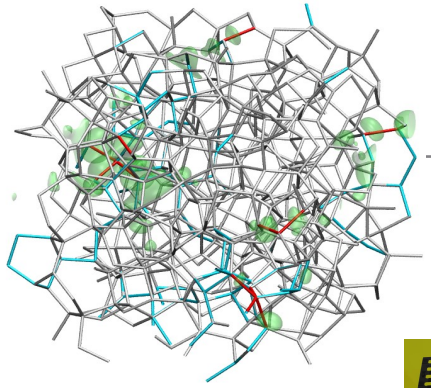


- Materials for Novel Dielectrics
  - Physical Review Letters 92, 146401 (2004)
  - Physical Review Letters 94, 236405 (2005)
  - Physical Review Letters 98, 037602 (2007)

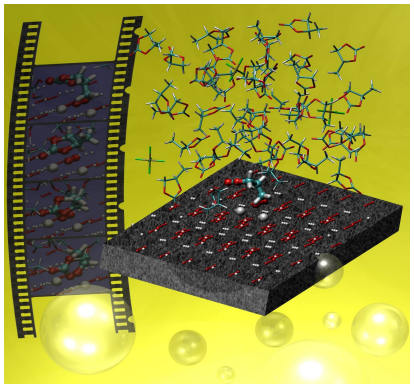


- Degradation of Coffee Aroma
  - with Nestle's Reseach Center
    J. Agr. Food Chem. (ACS) 51, 10 (2005)

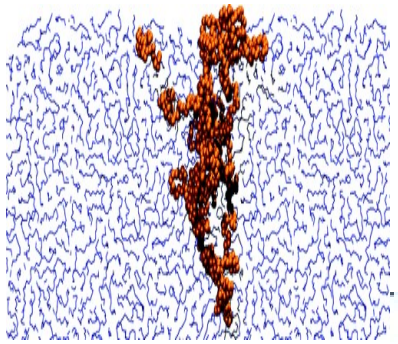
Real Examples



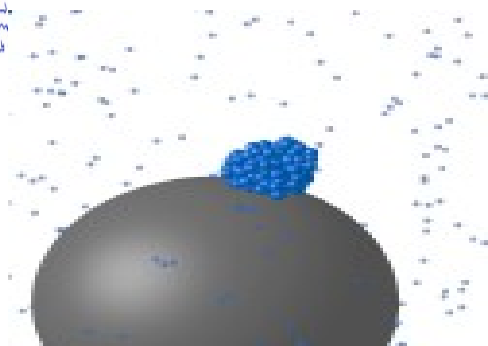
- a-Silicon Photovoltaics
  - Physical Review Letters 107,255502 (2011)



- Li-Air Batteries
  - Chemistry: A European Journal 18, 3510 (2012)



- Materials for High Voltage Insulators
  - with ABB Research
  - J. Phys. Chem. 115,2831 (2011)
  - J. Phys. Chem 115, 13508 (2012)



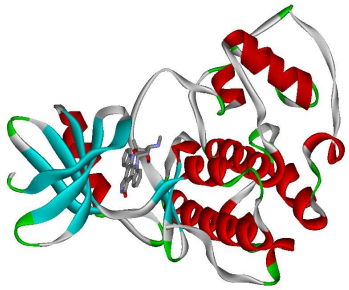
- Evolution and Degradation of Aerosols
  - with PMI research

    J. Phys. Chem. 115, 3592 (2012)

Real Examples

- Quantum Refined Scoring Function for Drug Design
  - with Novartis

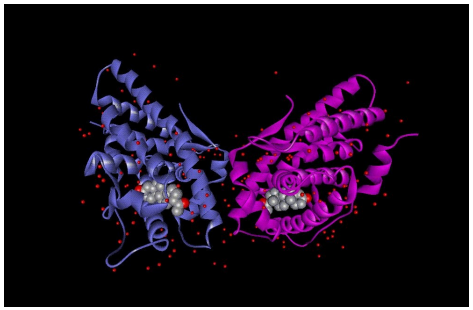
    J. Chem. Inf.and Mod. (ACS) 46, 254 (2006)



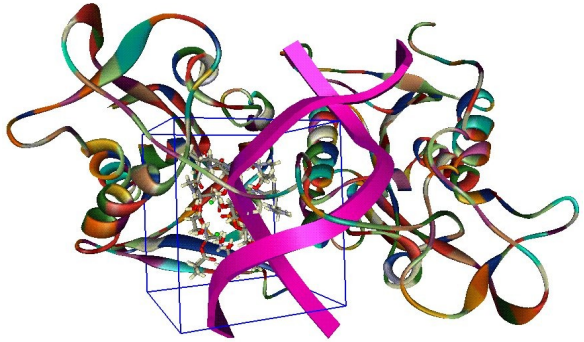
- Ligand-Protein interaction with QRFF
  - with Organon, Telethon Institute and S. Raffaele Hospital

    Chem Bio Chem 4, 155 (2003)

    Chemical Physical Letters 456, 236 (2008)



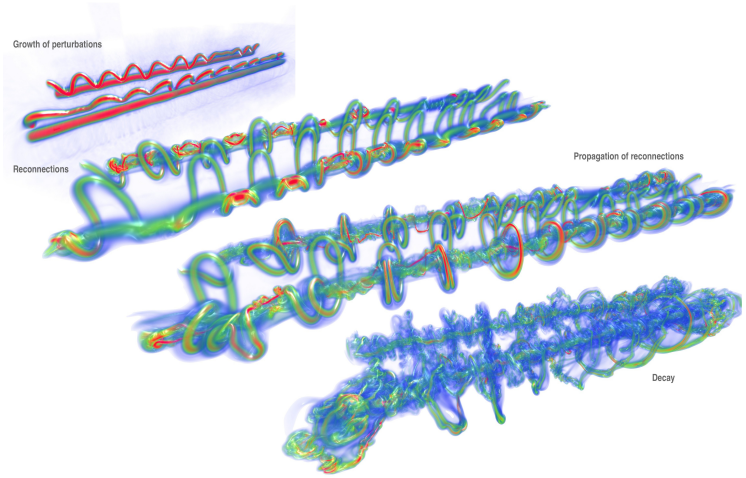
- QM/MM Modeling of Enzymatic Reactions
  - Journal of Biological Chemistry 278, 4381 (2003)



Real Examples

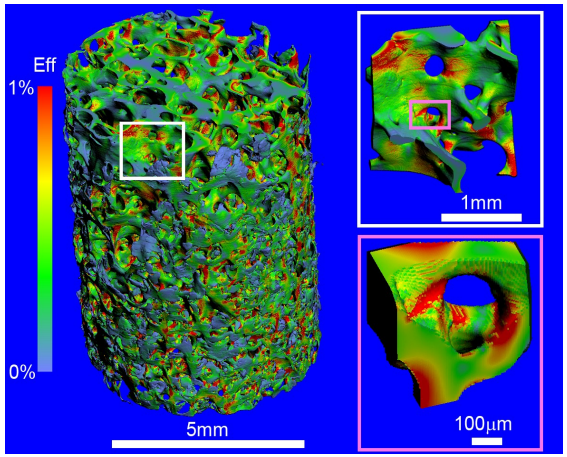
- DNS – CFD Simulations of Aircraft Trailing Vortices
  - with ETH – Prof. Koumoutsakos

    Comp. Meth. in App. Mech. and Eng.197, 1296 (2008)

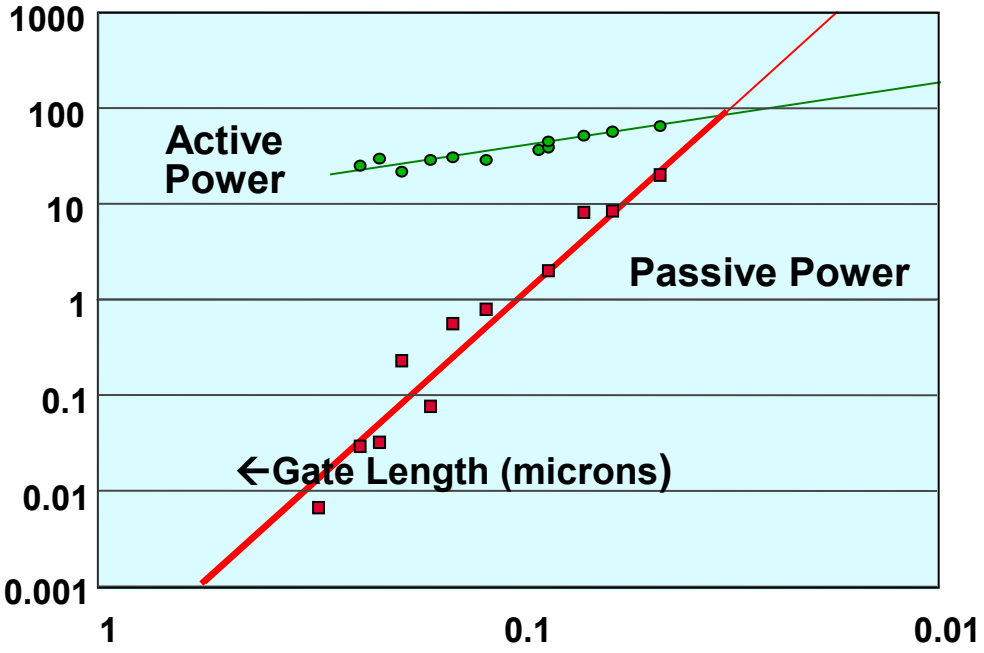


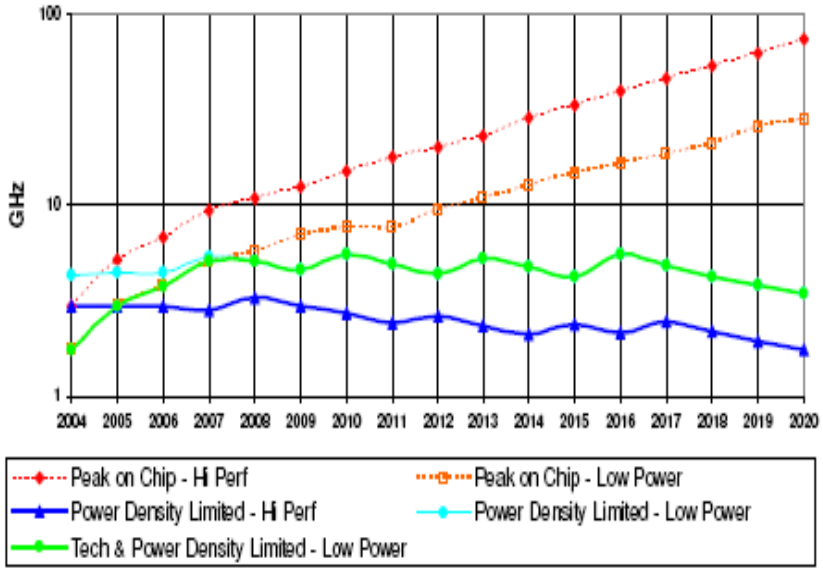
- μ-FEM Simulations of Bone Structures
  - with ETH – Prof. Mueller

    Concurrency and Computation: Practice and Experience, Wiley (2009)



The Origin of the Problem : End of CMOS Real Scaling

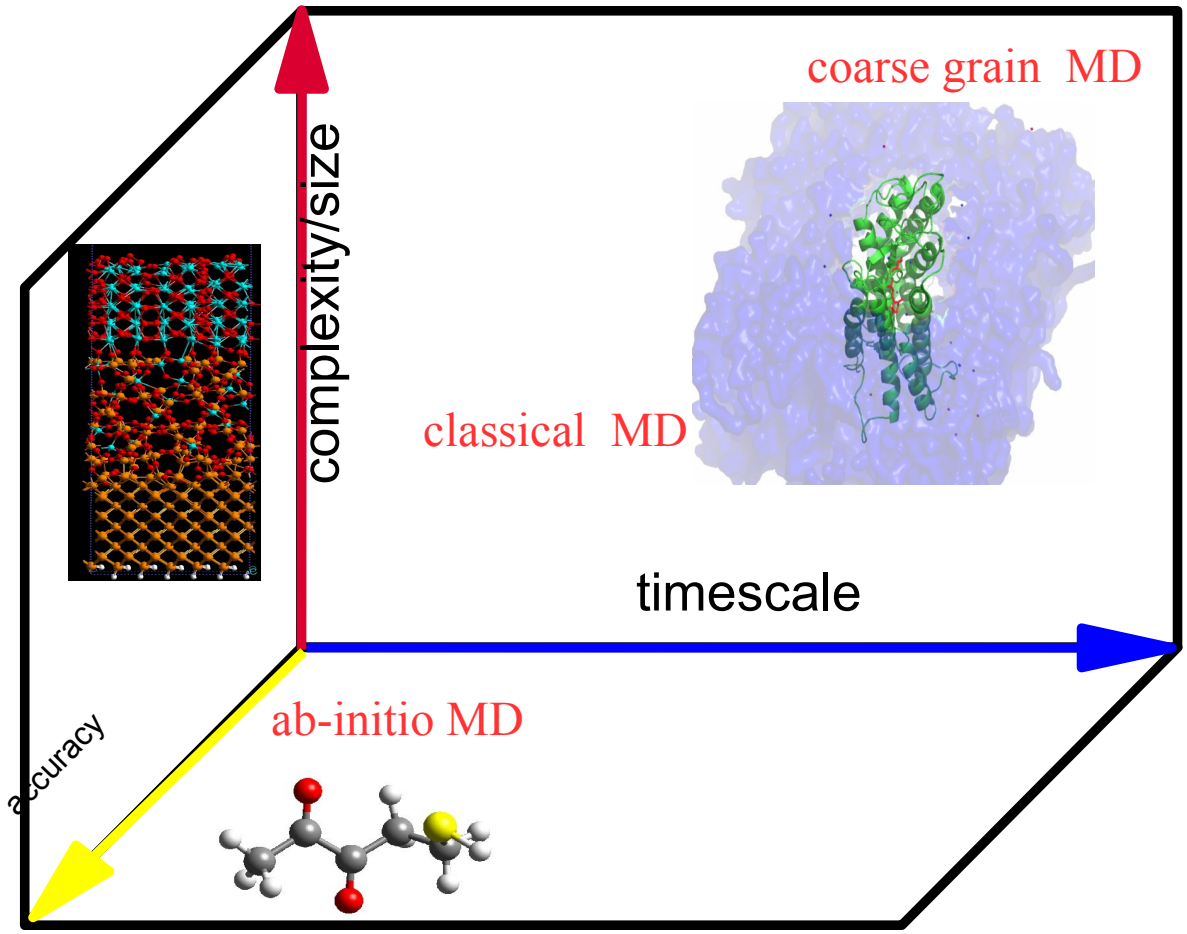




DARPA Report on Exascale (2008)

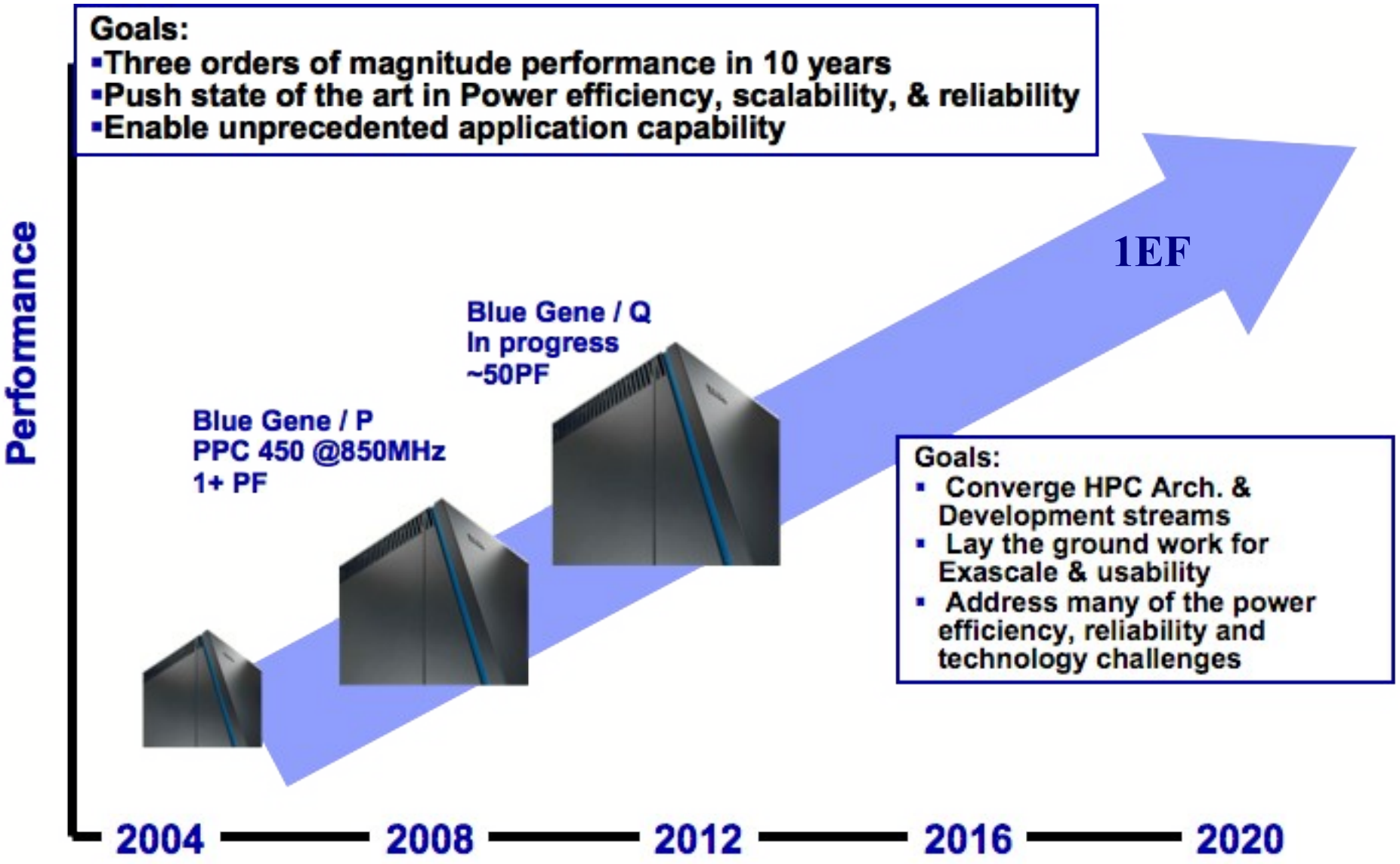
Most of the exponential increase in supercomputer speed is due to massively parallelism: 1 processor in 1990 - ~300'000 in 2010

The Spectrum of Atomistics Simulations



Computational Complexity and the number of Algorithmic Dwarfs playing a key role increase with the accuracy of the methods used.

BlueGene Evolution:



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  - CPMD parallelization and scaleout
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- The new challenges toward exascale computing
  - Fault tolerant and energy efficient algorithms
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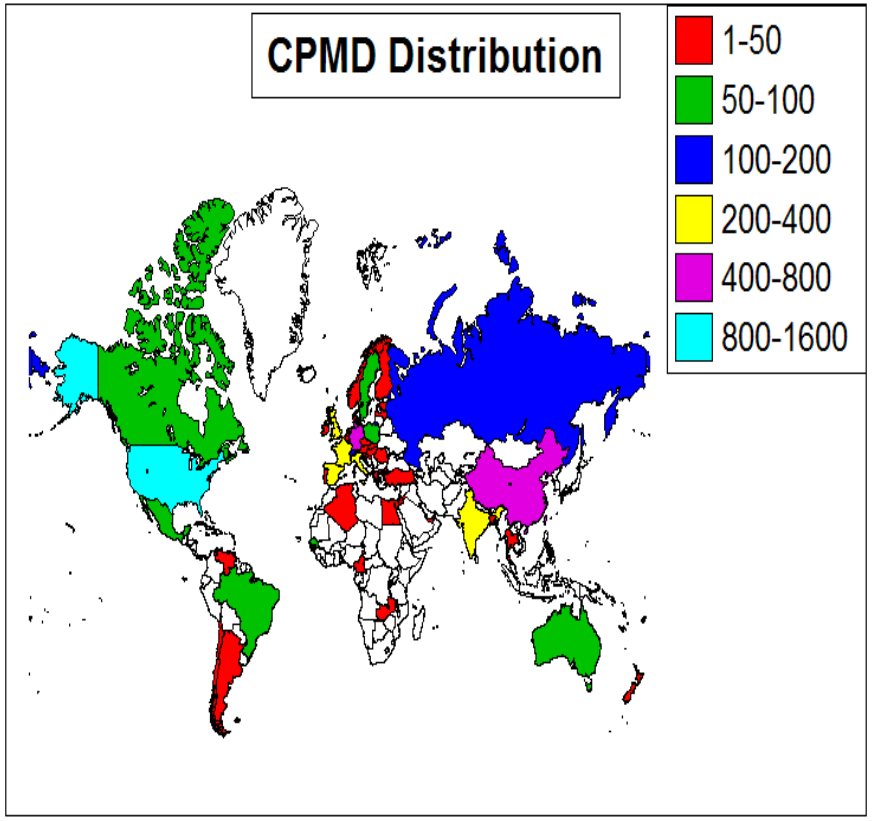
CPMD code history

- Born at IBM Zurich from the original Car-Parrinello Code in 1993 (J. Hutter) - implement DFT in the plane waves / pseudopotentials framework;
- developed in many other sites during the years; it has many unique features, e.g. path-integral MD, QM/MM interfaces, TD-DFT, LR calculations, metadynamics;
- since 2001 distributed free for academic institutions (www.cpmd.org);
- Major Contributors : M. Parrinello, J. Hutter, A. Curioni , M. Boero, D. Marx, P. Focher, M. Tuckerman, W. Andreoni, E. Fois, U. Roetlisberger, P. Giannozzi, T. Deutsch, A. Alavi, D. Sebastiani, A. Laio, A. Seitsonen, S. Billeter, A. Kohlmeyer, I. Tavernelli, N. Nair, D. Sebastiani, M. Iannuzzi, R. Vuilleumier, T. Laino, C. Bekas, V. Weber

The CPMD code: some facts

- Version 3.15.3:
- 10000+ licenses (www.cpmd.org) in more than 50 nations
- 1500+ members of the cpmd mailing list
- 3000+ publications (since 2001)
- More then 30000 citations



- Scalability up to 1Mthreads nodes
- 1 ns/week on 100 atoms system
- ~2000 molecules/day BG/P Rack
- Largest calculation: ~20000 atoms

- Used widely as benchmark for HPC
- Many of the algorithms innovations/concepts set the standard in the community

The evolution of ab-initio MD at ZRL

Year	System (limit)	Type of calculation	HW	Type of algorithm
1992	one organic molecule of ~50 atoms	dynamics; electronic structure	RISC6000/580 **(125 MFlops)**	serial
1994	liquid 100 atoms. organics water	reaction dynamics - free energy	SP1-16 nodes **(2 GFlops)**	parallel/MPI
1996	biomolecules 200 atom models *and in water*	reaction dynamics; electronic structure	SP2/66MHz 16 nodes **(4.2 GFlops)**	parallel/MPI
1998	complex interfaces 400 atoms. *water/oxide organic/metal*	all of the above	SP2/166MHz 32 nodes **(20.5 GFlops)**	parallel/MPI
2000	supramolecular systems 1000 atoms. *2D quantum dots arrays*	all of the above	SP3/200MHz 64/2 ways nodes **(102.4 GFlops)**	parallel/MPI+ OpenMP
2002	small proteins realistic interfaces 2000 atoms	all of the above	p690/1.3GHz 8/32 ways nodes **(1.3 TFlops)**	parallel/MPI+ OpenMP
2006	complex systems 5000 atoms	all of the above	2 BG/L Racks 4096 processors (11TFlops)	parallel/MPI+ taskgroup+
2008	complex systems 8000 atoms	all of the above	2 BG/P Rack 8192 processors (26 TFlops)	parallel/MPI+ taskgroup+ OpenMP

Total Energy of a molecular system

(Khon-Sham formulation of DFT in the BO approximation)

$$E_{tot}(R,r)=E_{el}(r;R)+E_{ion}(R)$$

$$E_{el}(r;R)=E_k+E_{ext}+E_h+E_{xc}$$

$$n_e(r)=\Sigma_\iota\ f_i\ |\Psi_\iota|^2$$

$$E_k=-1/2\ \Sigma_i <\Psi_\iota \mid \Delta \mid \Psi_\iota>$$ (Kinetic Energy)

$$E_{ext}=\int V_{ext}(r)n_e(r)dr$$ (Nuclei/Electrons interaction Energy)

$$E_h= 1/2\iint n_e(r_1)\ 1/r_{12}\ n_e(r_2)\ dr_1dr_2$$ (Hartree Energy)

$$E_{xc}= \int \varepsilon_{xc}(r)n_e(r)\ dr$$ (Exchange-Correlation Energy (*ManyBody Term*))

Total Energy of a molecular system with a plane wave basis set

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}} c_i(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}}$$

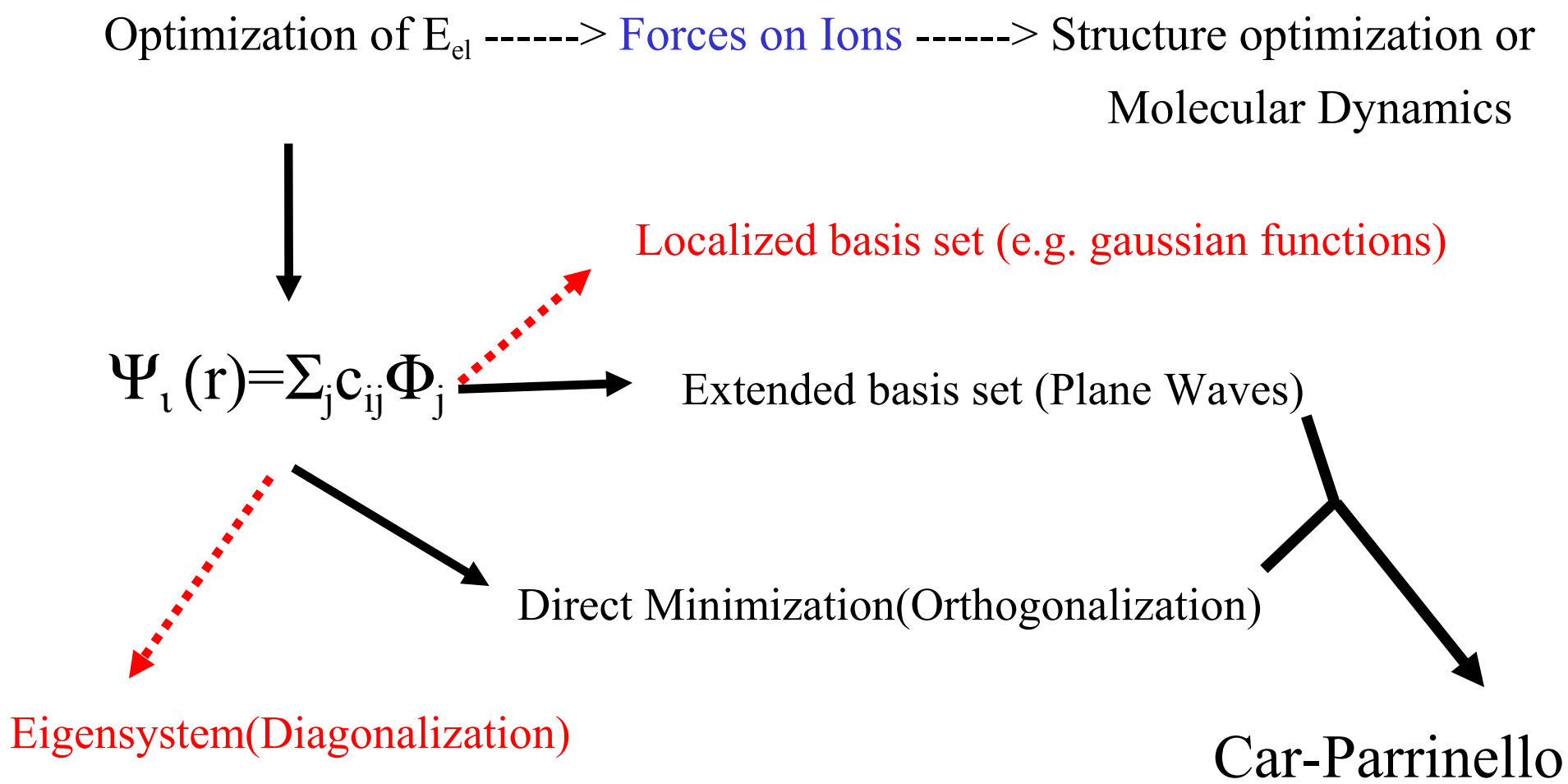
$$n(\mathbf{r}) = \sum_i f_i \left|\psi_i(\mathbf{r})\right|^2$$

$$E_{kin} = \frac{1}{2} \sum_i f_i \sum_{\mathbf{G}} \mathbf{G}^2 \left|c_i(\mathbf{G})\right|^2 \qquad E_{loc} = \Omega \sum_{\mathbf{G}} n^*(\mathbf{G}) S(\mathbf{G}) V_{loc}(\mathbf{G})$$

$$E_H = 2\pi\Omega \sum_{\mathbf{G}} n^*_t(\mathbf{G}) \frac{1}{\mathbf{G}^2} n_t(\mathbf{G}) \qquad E_{XC} = \frac{\Omega}{N} \sum_i \varepsilon(\mathbf{r}_i) n(\mathbf{r}_i)$$

$$E_{nl} = \sum_I \sum_j f_j \left|F_j^I\right|^2$$

Optimization of Molecular Structure



Scaling I

The size of a system is determined by the number M of PWs needed for its accurate description, the number N of electrons, and the number I of ions.

Electronic minimization:

(CPU time)

-NMlogM (e.g. calculation of the density, calculation of the forces)

-N^2MlogM (e.g exact exchange)

-N^2M (e.g. orthogonalization)

(Memory)

-NM (electronic wavefunction in reciprocal space)

Scaling II

Structure minimization:

(CPU time)

$-I^3$ (BFGS)

(Memory)

$-I^2$ (Hessian)

For most systems:

$M>>>N>I$

Simulation time dominated by 3D-FFTs for systems <1000 atoms

by Orthogonalization for systems > 1000 atoms

CPMD Parallelization & Scale out

- **Distribute plane waves and parallelize 3D-FFT (MPI API)**
  - maximum scaling 128 procs - 400 atoms
- **Mixed MPI/OpenMP parallelization**
  - maximum scaling 1024 procs -1000 atoms

  J. Hutter and A. Curioni, Parallel Computing (31) 1, 2003
- **Hierarchical Taskgroup parallelization for BG**
  - Extreme scale-out 128K procs – 110 TFlops

  G. Almasi, A. Curioni et al, IEEE Comp. Soc. 57 (2004)

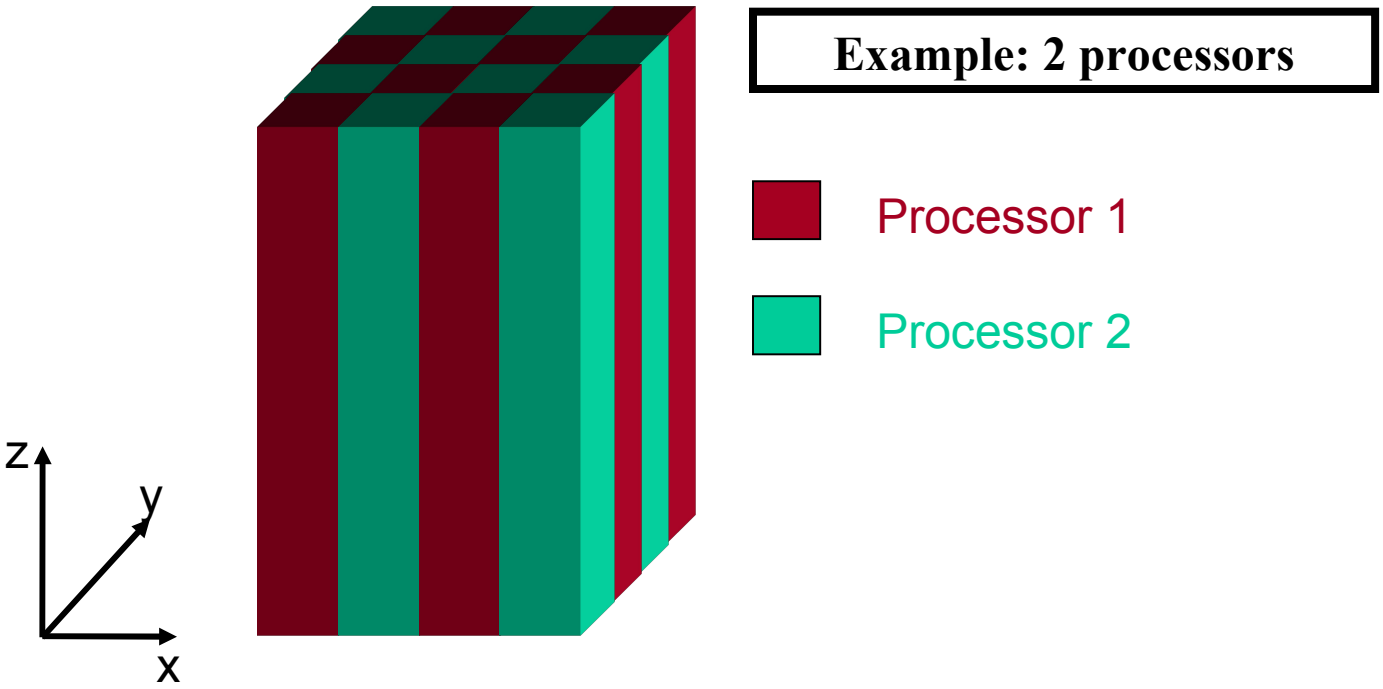
  J. Hutter and A . Curioni, Chem Phys Chem (6):1788-1793 (2005)
- **Parallel Linear Algebra and Parallel Initialization**
  - >10000 atoms **(8K atoms demonstrated on 4 Racks)**

  C. Bekas and A. Curioni, Parallel Computing (34): 441-450 (2008)
- **Cache/Network Optimized Orthogonalization**

  C. Bekas and A. Curioni, Comp. Phys. Comm. (181) 1057-1068 (2010)

Distributed Memory 3D FFT

For each wave function: Distribute its coefficients over the G-vectors across the z-direction, thus forming "pencils"



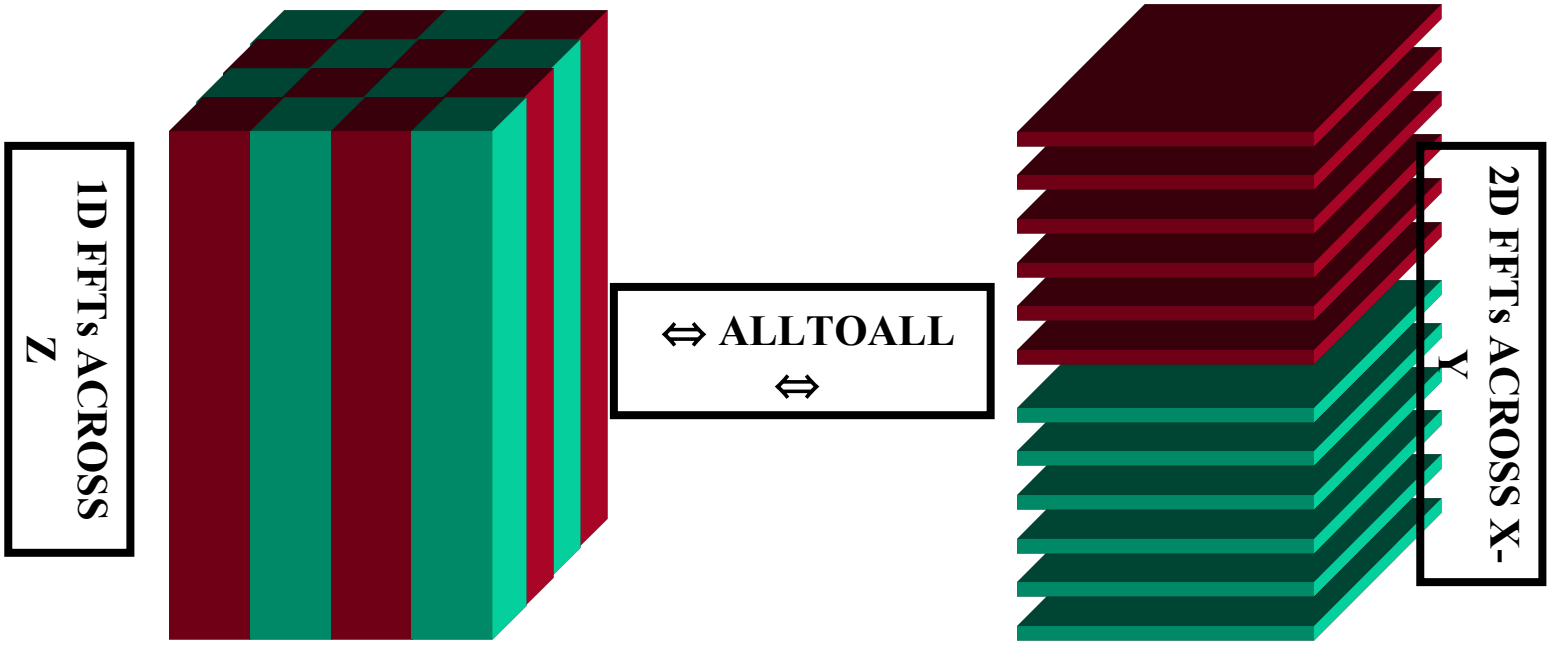
Distributed Memory Implementation in CPMD

3D FFT: can be computed in 3 steps

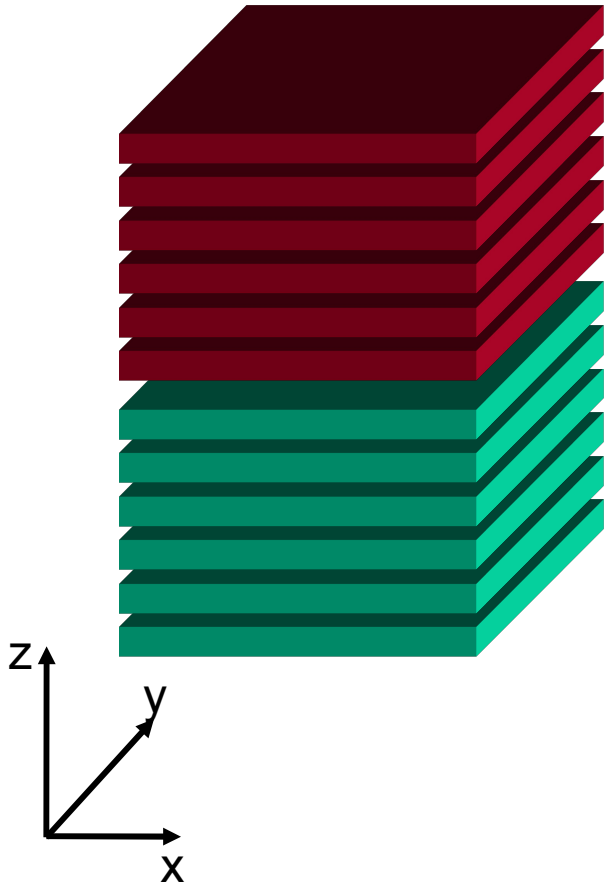
1D FFT across Z ⇒ 1D FFT across Y ⇒ 1D FFT across X

…or 3D FFT in two steps

1D FFT across Z ⇒ 2D FFT across X-Y planes



Limited Scalability of Standard 3D FFT



Each processor takes a number of whole planes…

Very good scheme for small – medium sized computational platforms…but

Observe that scalability is limited by the number of planes across the Z-direction! ... Which is in the order of a few hundreds… O(100)…

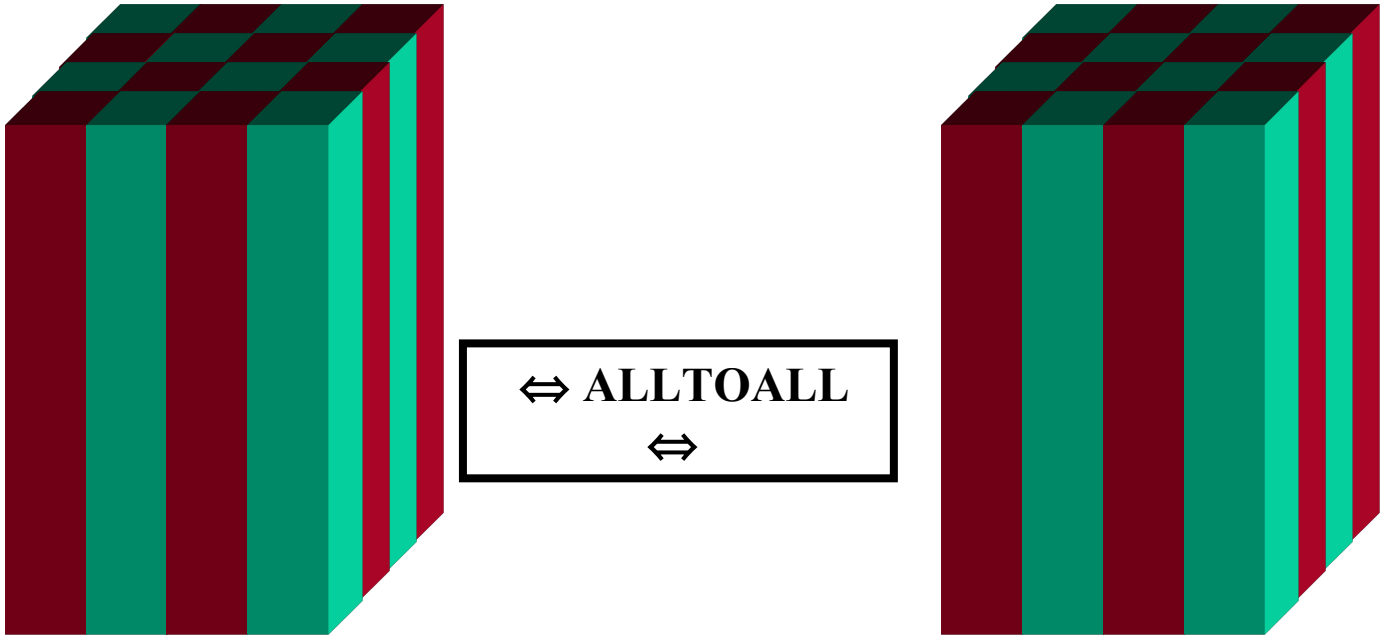
Thus: not appropriate for extreme scaling

3D FFT Using Task Groups

$$\rho(r) = \sum_{occ} |\psi_i(r)|^2$$

Loop across the number of electrons. Each states requires one 3D FFT.

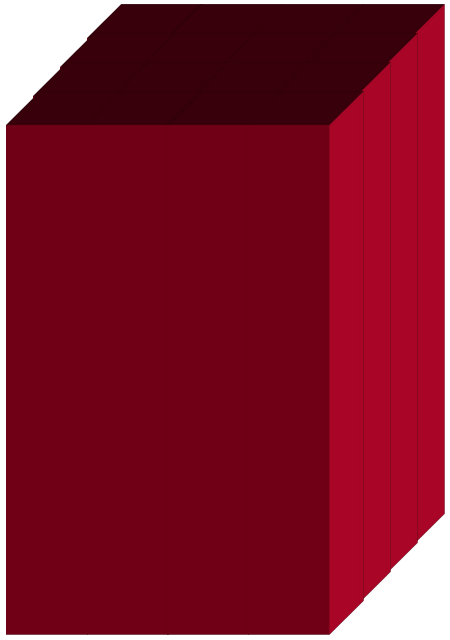
Hierarchical parallelism*: Assign to each Task Group a number of states.



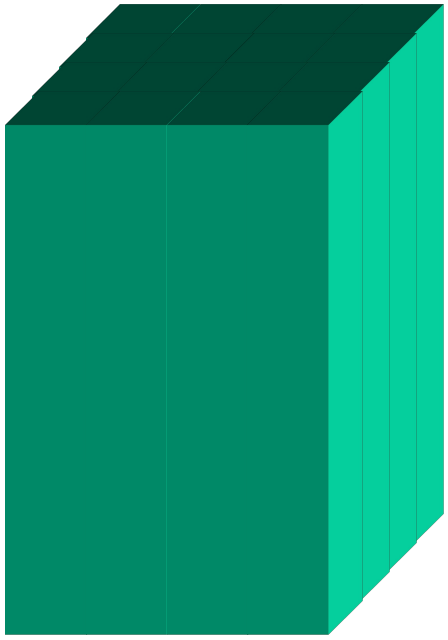
* J. Hutter and A. Curioni, Parallel Computing (31) 1, 2005

3D FFT Using Task Groups

- **The Task Groups of processors will work on different eigenstates concurrently**
- **Number of processors per group: Ideally the one that achieves the best scalability for the original parallel 3D FFT scheme**



EIG 1: ONLY PROC 1



EIG 2: ONLY PROC 2

Exact Exchange – Gamma Point Parallel Implementation

$$E_{x-exact}[\{\psi\}] = -\frac{1}{2\Omega}\sum_{\sigma=\uparrow,\downarrow}\left(\frac{\Omega}{8\pi^3}\right)^2 \int_{BZ} d\mathbf{k} \int_{BZ} d\mathbf{l}$$
$$\times\left[\sum_{n=1}^{N_{occ}^{\sigma}}\sum_{m=1}^{N_{occ}^{\sigma}}\sum_{\mathbf{G}}\frac{4\pi}{|\mathbf{G}-\mathbf{k}+\mathbf{l}|^2}\rho^{\sigma}_{ml;nk}(-\mathbf{G})\rho^{\sigma}_{nk;ml}(\mathbf{G})\right]$$

F. Gygi and A. Baldereschi Phys Rev Lett 62, 2160 (1989),
P. Broqvist, A. Alkauskas, and A. Pasquarello Phys. Rev. B 80, 085114 (2009)

NEW TASKGROUP STRATEGY

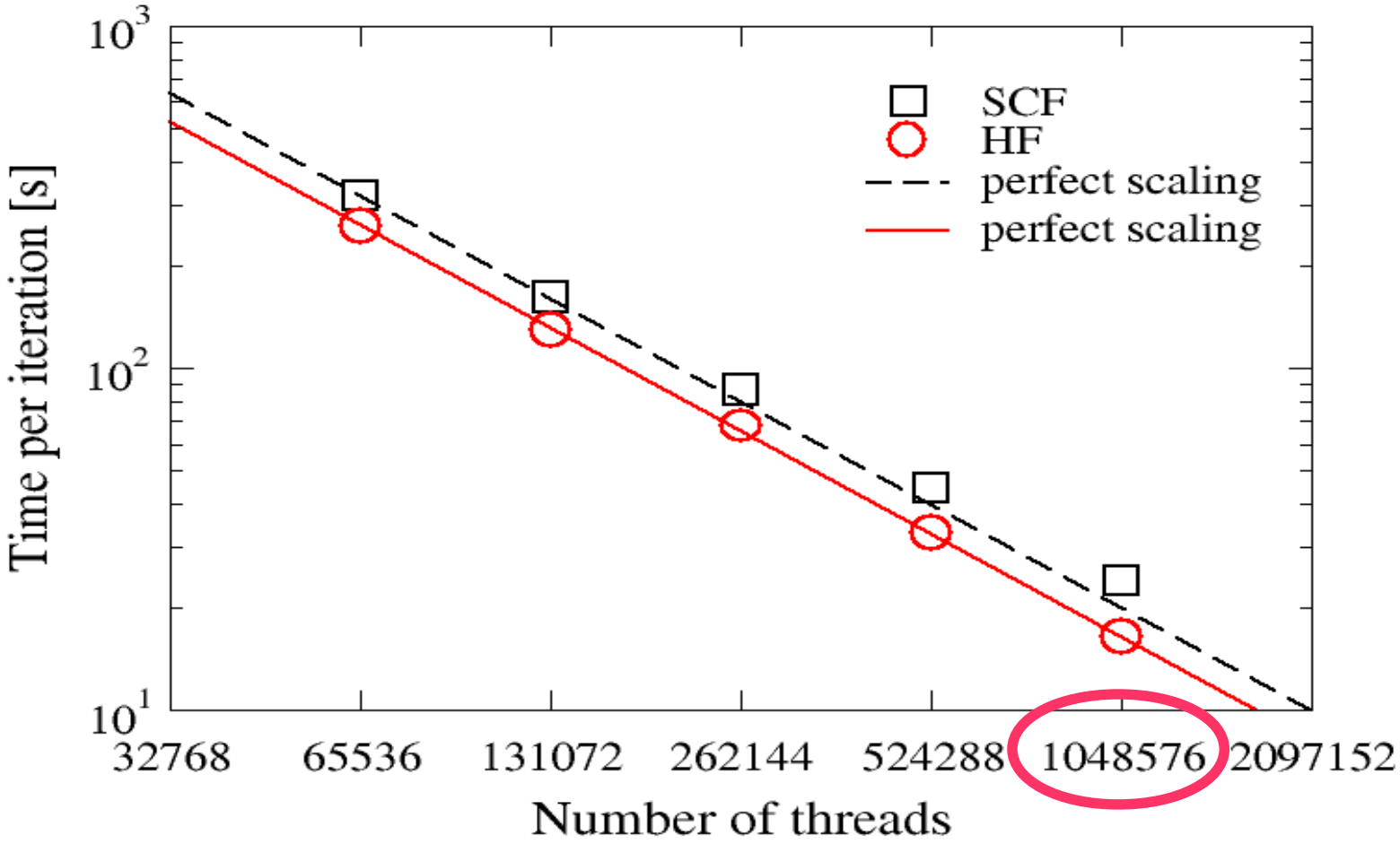
Distribute States and Orbital Couples

Exact Exchange: (~ N^2 MlogM)

- each group computes a subset of the orbital (non redundant) pairs
- cyclic distribution of the pairs (scalapack like) – with dynamic balancing
- the X-energy and the X-contribution to the electronic gradient are summed/redistributed at the end of the computation (inter groups communication)
- possible thresolding via orbital localization and overlap densities estimation

LATEST BG/Q Results

Implementing Exact-Exchange in CPMD
>95% Parallel Efficiency to over 1M threads



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Original CPMD Orthogonalization

The Cholesky based orthonormalization

1) Matrix X (Electronic States) is distributed row wise

2) Calculate distributed overlap matrix $S = X^T X$ — **BLAS 3. Global reduction needed**

3) Compute parallel Cholesky decomposition $S=R^TR$ — **BLAS 3.Send/Recv**

4) Invert triangular matrix R. R^{-1} is distributed — **BLAS 3. Send/Recv**

5) Compute orthonormal vectors $Y=XR^{-1}$ — **BLAS 3. Many Broadcasts**

Original CPMD Orthogonalization

Computational aspects and practical parallel deployment in *ab initio* codes

- ✓ **BLAS 3. Performance and Cache optimized-**
- ✓ **Numerical stability problems? Not really…**

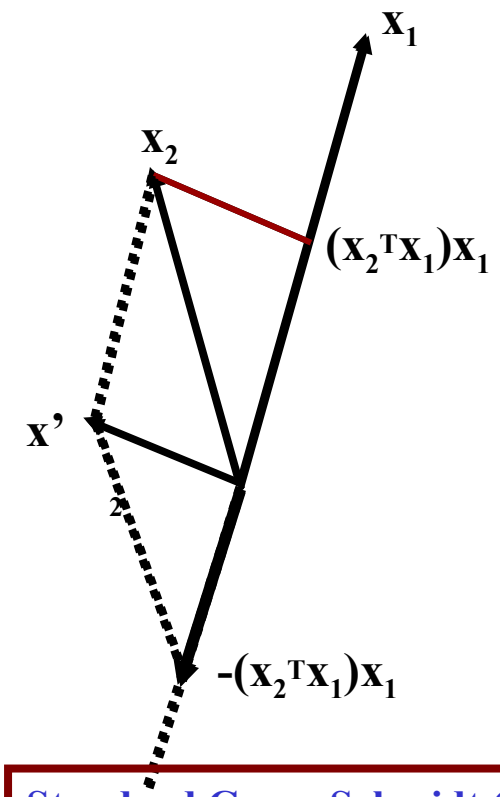
Then what is the catch? …Consider massively parallel deployment!
(++thousands of procs)

\+ **Matrix X (wavefunctions) is distributed row-wise to all available procs. So, the calculation of the overlap matrix $S = X^T X$ will scale**

\- **But then the overlap matrix can have less rows (columns) than the available procs!**
\- **Very difficult to scale.**
\- **Not optimized in terms of communication needs and Network Topology**
  - **Typical overlap matrix sizes: 100 (small), 500 (medium), 2000 (large), 10000 (very large)**
  - **Typical massively parallel deployment: 10s to 100s of thousands of proc elements**

SCALAPACK like scaling stops at hundreds of procs.

How about Gram-Schmidt?



$x_1 = x_1/||x_1||$

for i=2,…,k

$w(1:i-1) = X(:,1:i-1)^T x_i$

BLAS 2. Global reduction needed

for j=1:i-1

$x_i = x_i - w(i)*x_j$

BLAS1. No communication needed

end

$x_i = x_i/||x_i||$

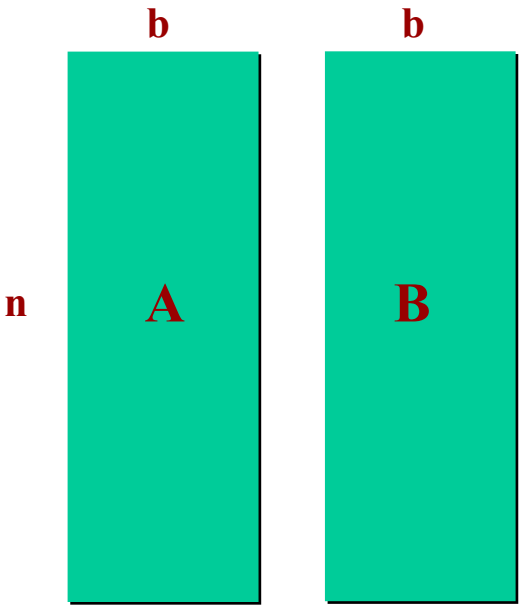
BLAS 1. Global reduction needed

end

Standard Gram-Schmidt (Modified GS rarely needed in *ab initio*) will scale very well on massively parallel platforms with very fast collective communication networks (BG/P).

Scalar per node performance is low though because of BLAS 2 nature! Cost: $O(2nk^2)$

Our proposal: Block Gram-Schmidt!



Consider the n x b matrices A and B such that

- ✓ **A is orthonormal: $A^TA = I$**
- ✓ **B is not orthonormal: $B^TB \neq I$**

Then, if $W = A^TB$ we can subtract the "overlap" of B on A from B so that $A^TB = I$:

- ✓ **$B = B - AW$**

Observe: this a BLAS3 operation (DGEMM)

We then need to orthonormalize the new B:

- ✓ **We utilize the Cholesky based approach here**
- ✓ **Remember: we keep b small but large enough to yield good BLAS3 performance**

Generalizing the procedure yields Block Gram-Schmidt

Our proposal: Block Gram-Schmidt!

M = k/b /* Consider a block size b: O(100) */
for i=1,…,M

if i>1

$W(1:b,1:(i-1)*b) = X(:,1:(i-1)*b)^T X(:,(i-1)*b+1:i*b)$

BLAS 3. Global reduction needed

$X(:,(i-1)*b+1:i*b) = X(:,(i-1)*b+1:i*b) - \ldots$
$X(:,1:(i-1)*b) W(1:b,1:(i-1)*b)$

BLAS 3. No Global reduction needed

end

$S = X(:,(i-1)*b+1:i*b)^T X(:,(i-1)*b+1:i*b)$

BLAS 3. Global reduction needed

$R = chol(S)$

BLAS 3. Performed locally!

$X(:,(i-1)*b+1:i*b) = X(:,(i-1)*b+1:i*b) R^{-1}$

BLAS 3. No communication needed

end

Let's summarize

Matrix size: n x k, k << n

Cholesky based orthogonalization

- **Cost: $3nk^2$**
- **BLAS 3**
- **Difficult to scale on thousands of procs**

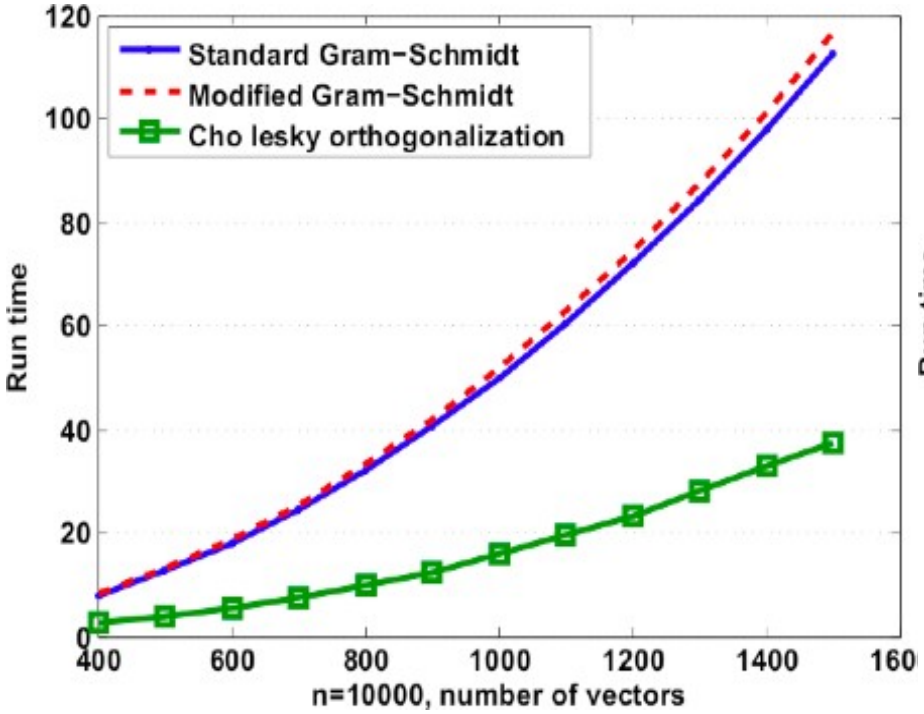
Gram-Schmidt

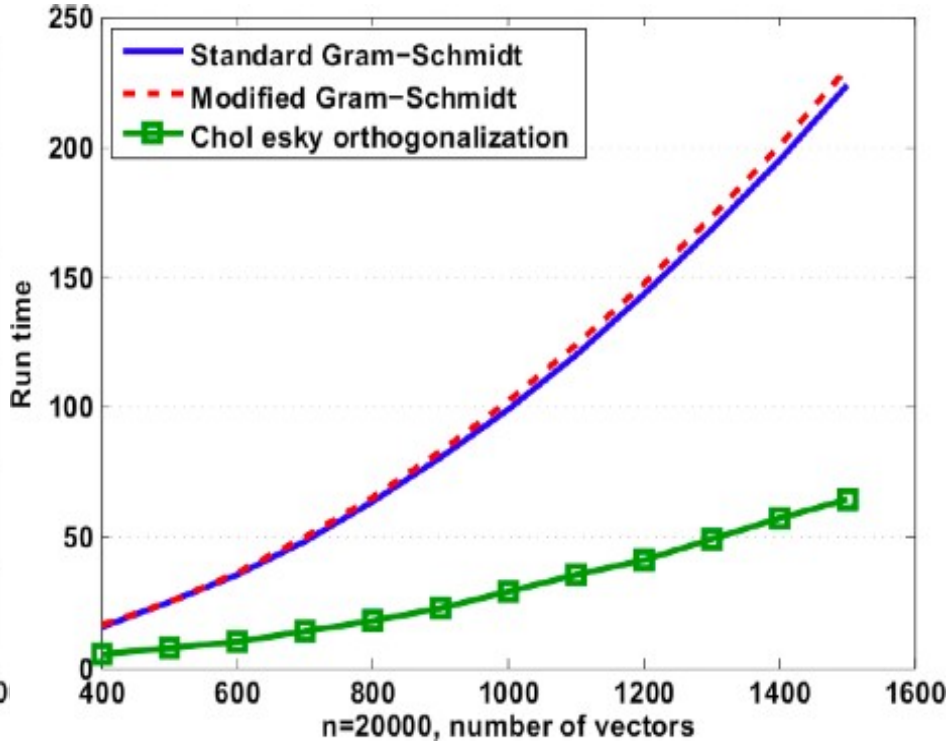
- **Cost: $2nk^2$**
- **BLAS 2**
- **Easier to scale. Very Low scalar performance**

Block Gram-Schmidt [Bekas-Curioni, CPC 181(6): 1057-1068 (2010)

- **Cost: $2nk^2$**
- **BLAS 3**
- **# of messages: O(k/b) [or O(k/b)^2 in the modified case]**
- **Cache optimized AND Network optimized**
- **Designed to inherit the strong points of preexisting schemes**

Tests: Gram-Schmidt v.s. Cholesky based

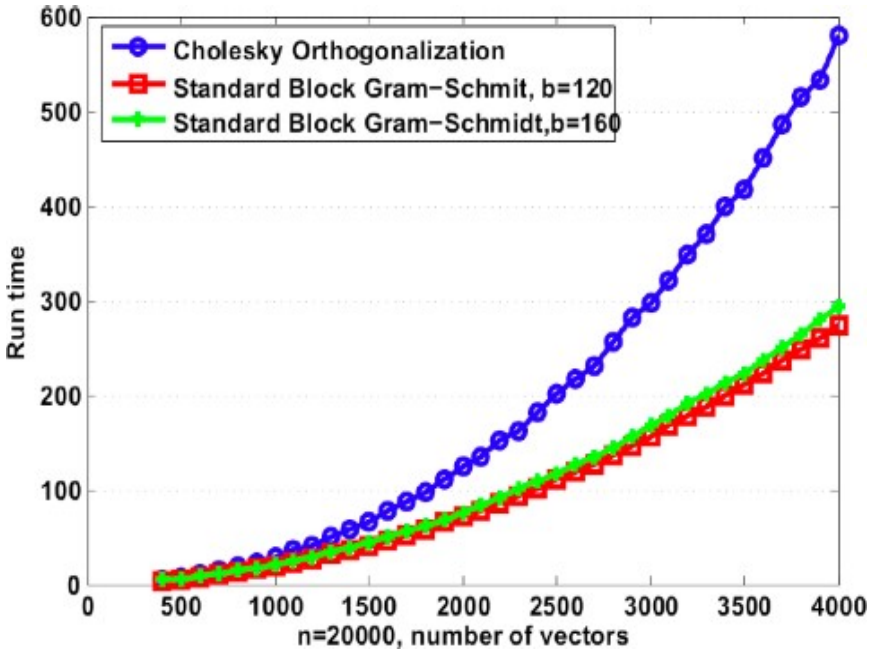


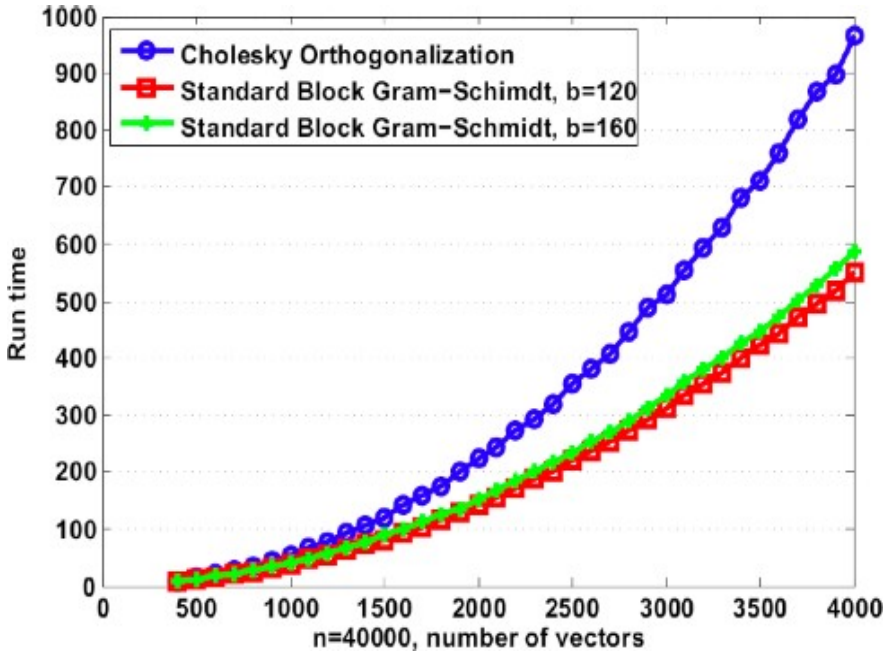


N=10000 (left) and N=20000 (right). Varying number of vectors to orthogonalize. Times in seconds

The BLAS3 based Cholesky approach although more costly than the BLAS1-2 based GS clearly wins

Tests: Block GS v.s. Cholesky based ortho

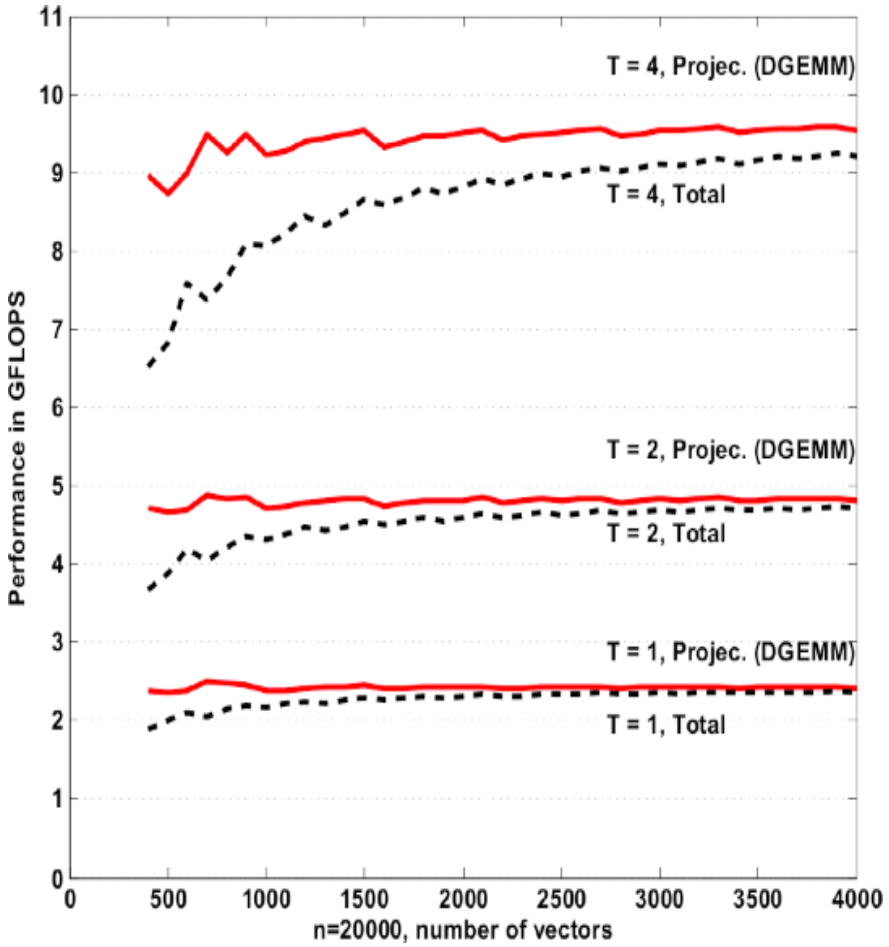


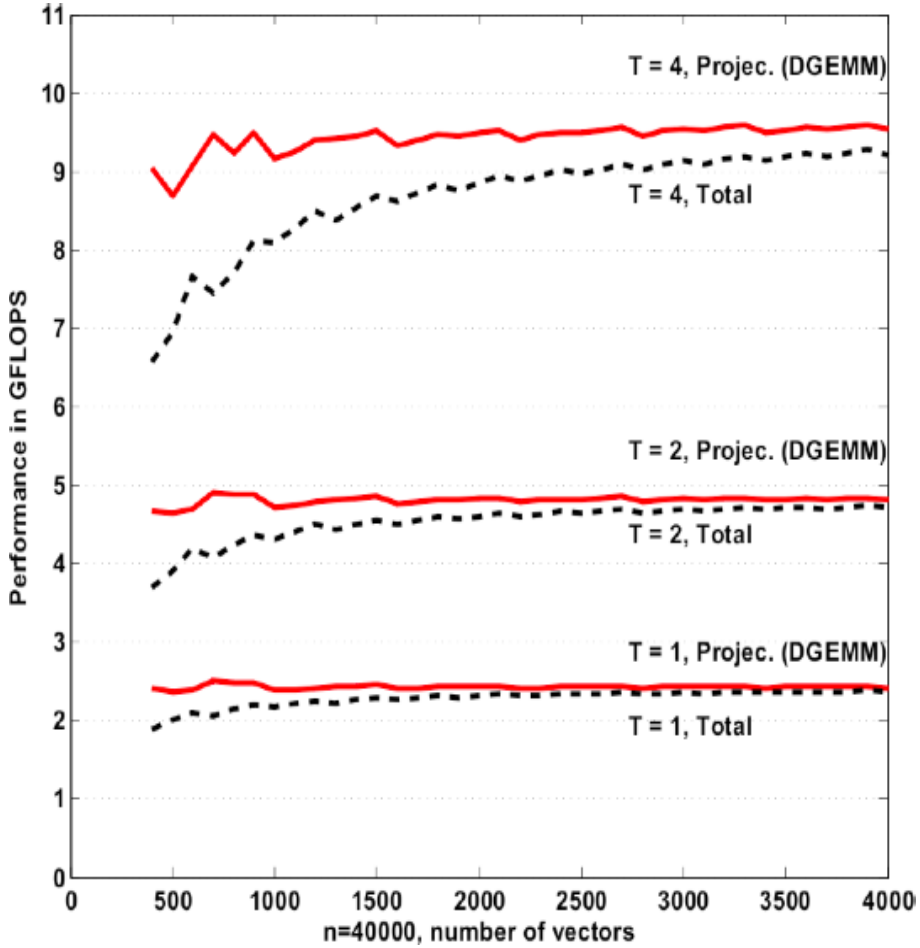


N=20000 (left) and N=40000 (right). Varying number of vectors to orthogonalize.

Comparison of Cholesky based v.s. Block (modified-standard) Gram-Schmidt (Run times in seconds)

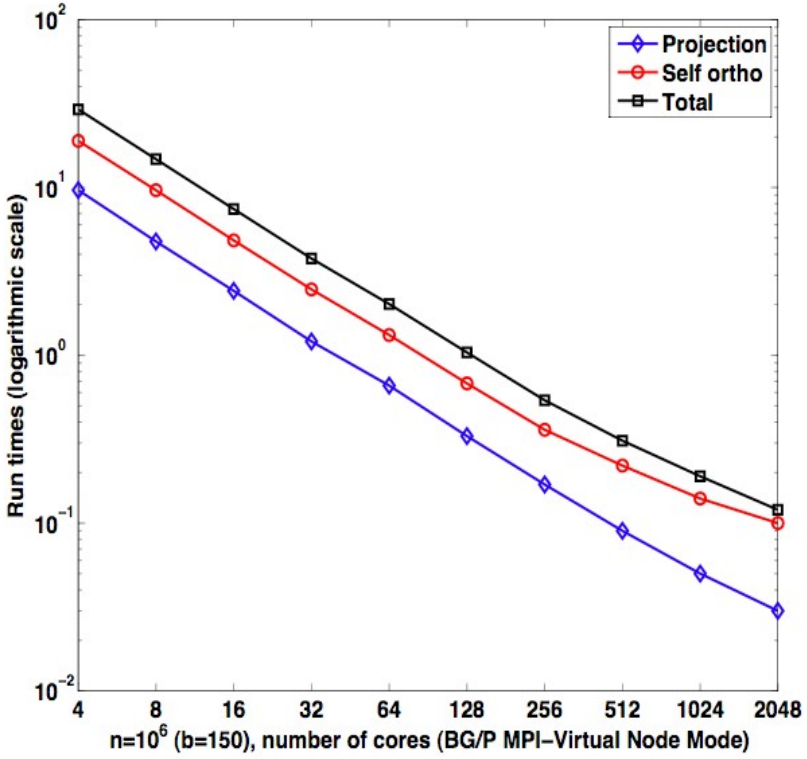
Block GS SMP parallelism



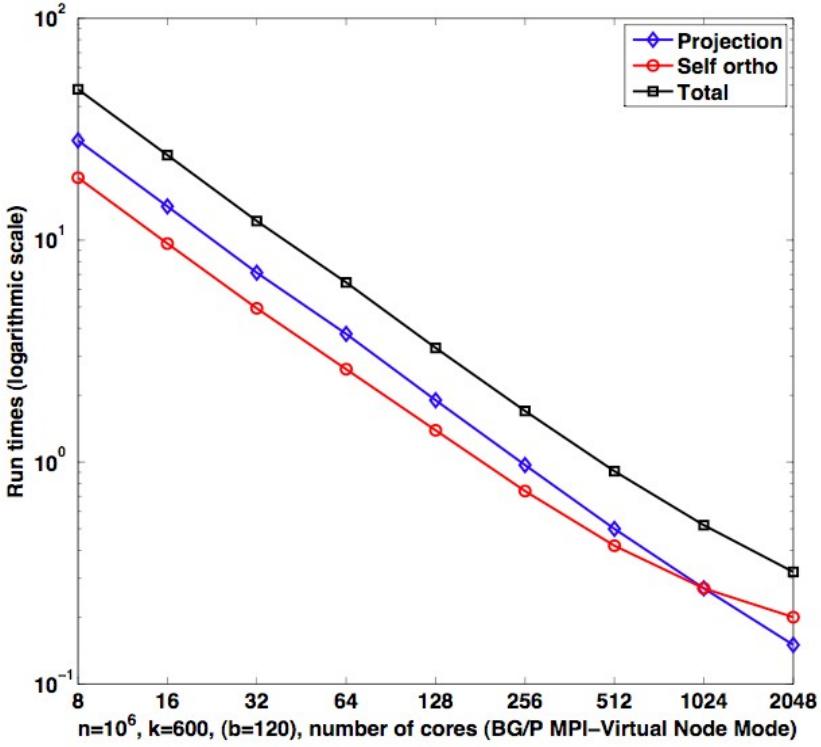


SMP Block GS. 1-4 threads (ESSL), blocksize b=120, left n=20000, right n=40000

Test: Block Gram-Schmidt - Scale-out

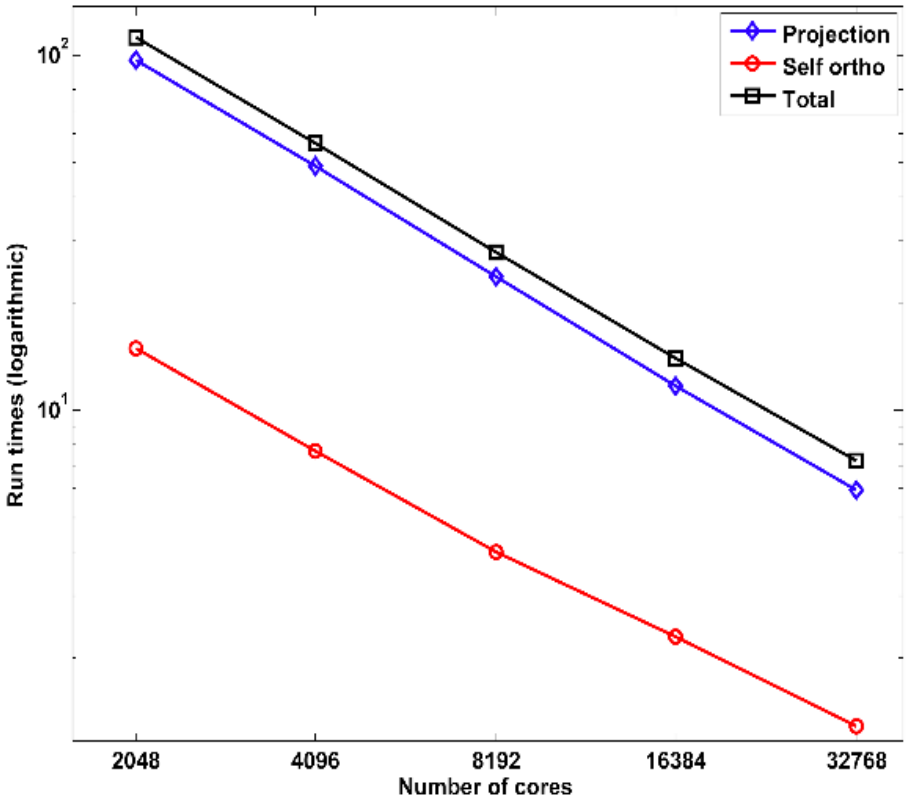


Run times: N=1M, k=300, log scale

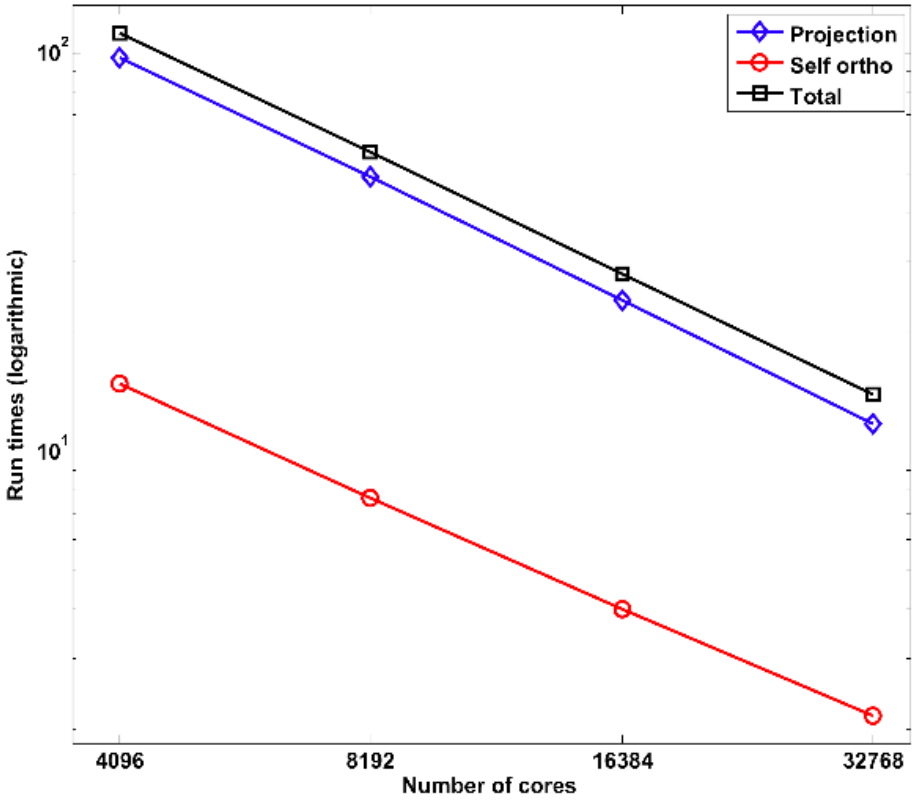


Run times: N=1M, k=600, log scale

Tests: Block Gram-Schmidt - Scale-out



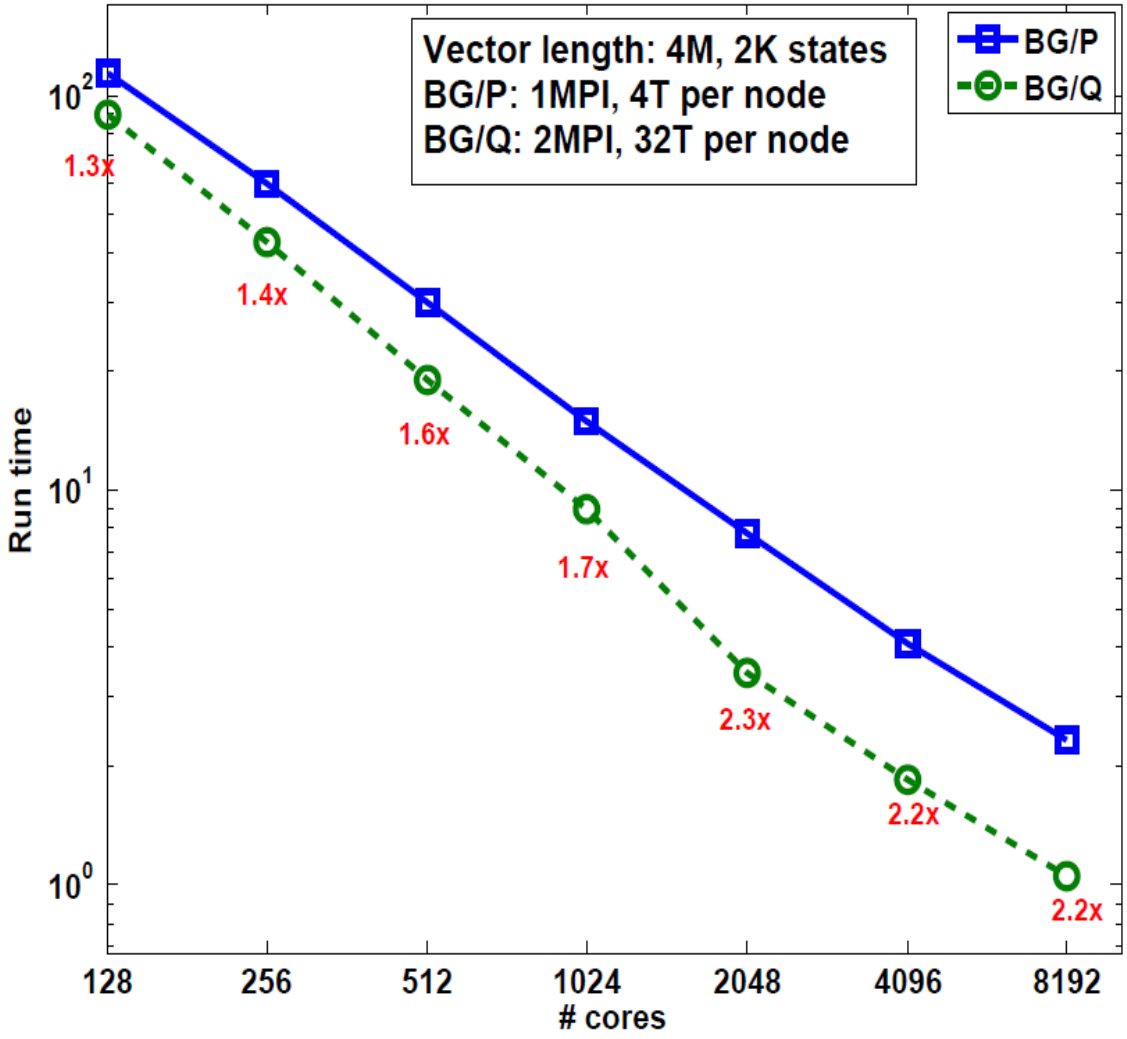
Run times: N=60M, k=2000, log scale



Run times: N=60M, k=4000, log scale

70% peak on 8 BG/P racks

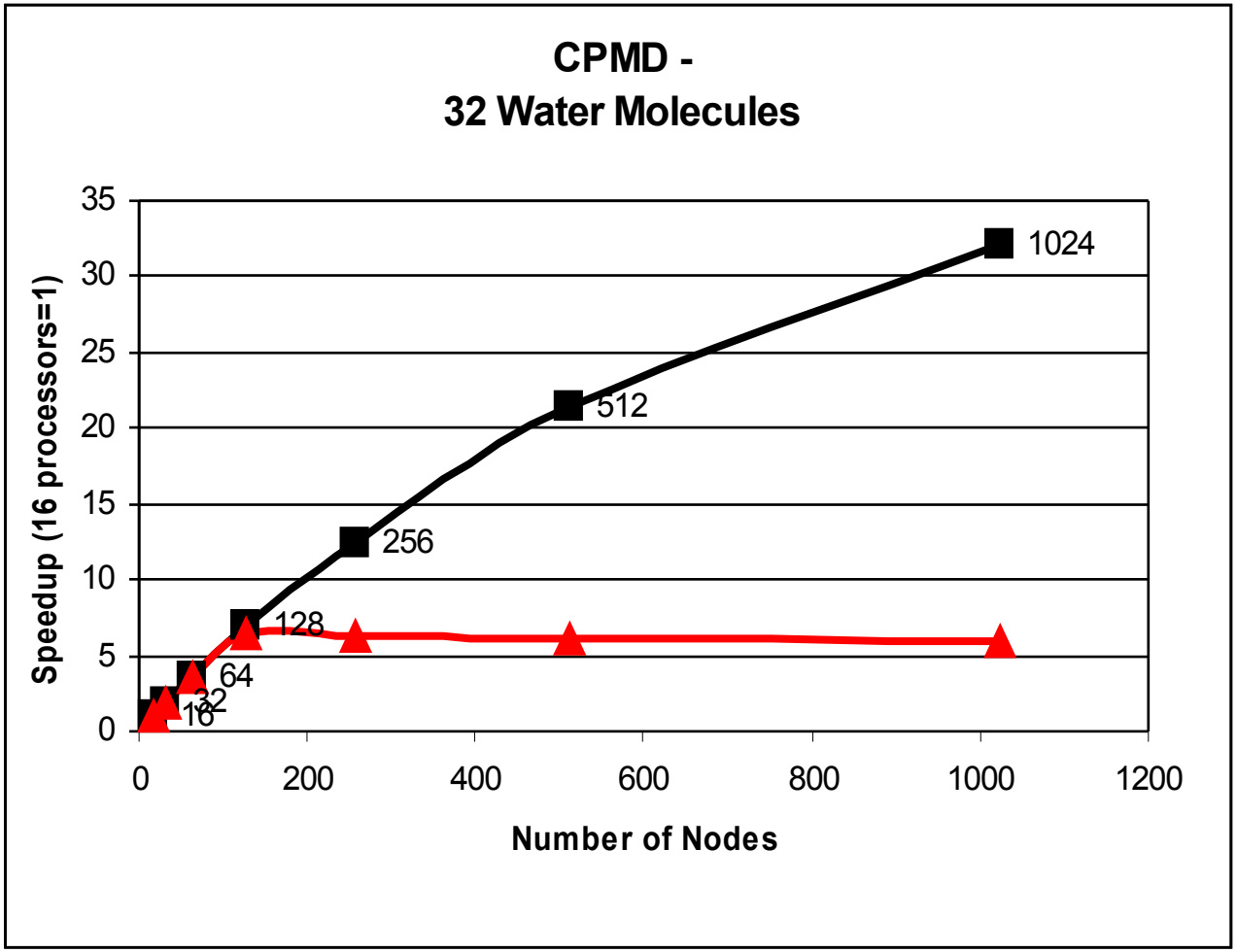
Tests: Block Gram-Schmidt - BG/P vs BG/Q



Test Cases

- **Test 1 :** 32 water molecules
  Cutoff 70 Ry – norm conserving pseudos
- **Test 2 :** 576/1576 atoms Propylene Carbonate/Li_2O_2
  Cutoff 100 Ry - norm conserving pseudos
- **Test 3 :** 1000-8000 atoms SiC
  Cutoff 35Ry – norm conserving pseudos
- **Test 4 :** ~600 atoms – Li_2O_2 PC – metadynamics
  Cutoff 70 Ry – norm conserving pseudos
- **Test 5 :** ~500 atoms – aSiH – hybrid functionals
  Cutoff 70 Ry – norm conserving pseudos

Test 1: 32 water (70Ry)

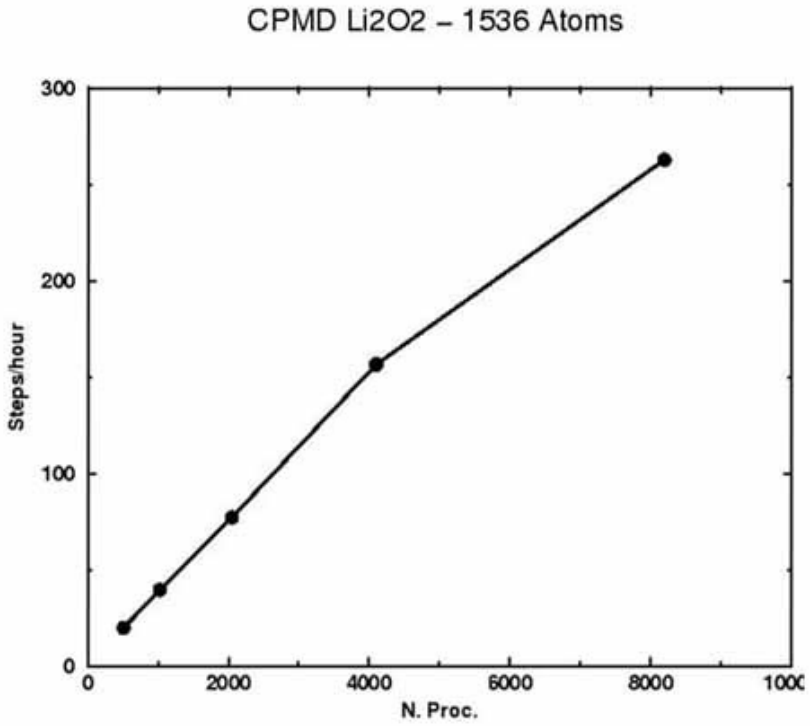


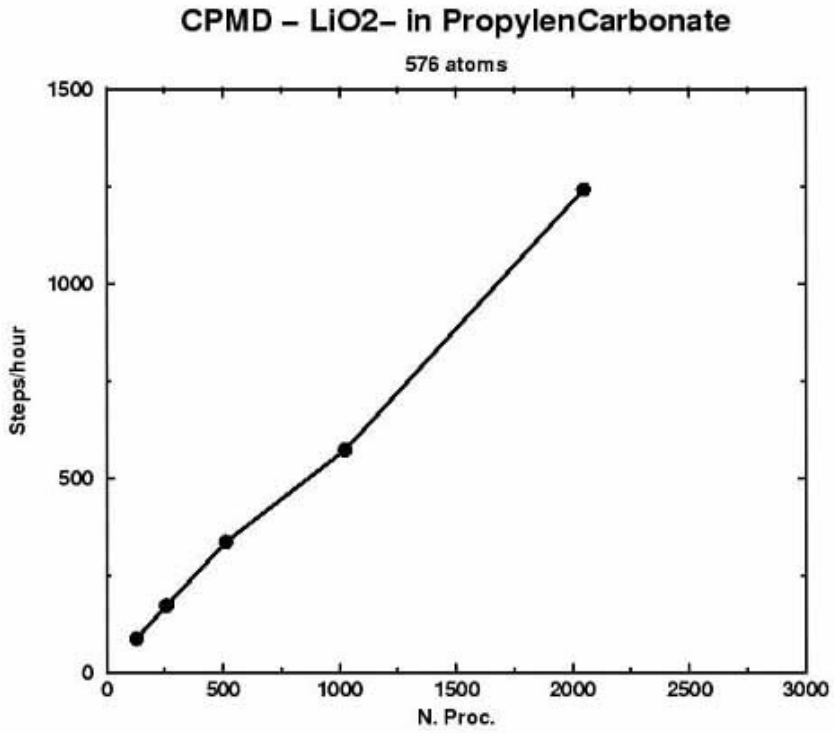
Single processor performance ~2.1 speedup after optimization

PWR7 4.0GHz
1.2 sec/step on 16 processors

Best Time per step = 0.09 sec on 2048 nodes
(red without taskgroups) ;~650 ps/week

Test 2: Li_2O_2 and Propylen Carbonate

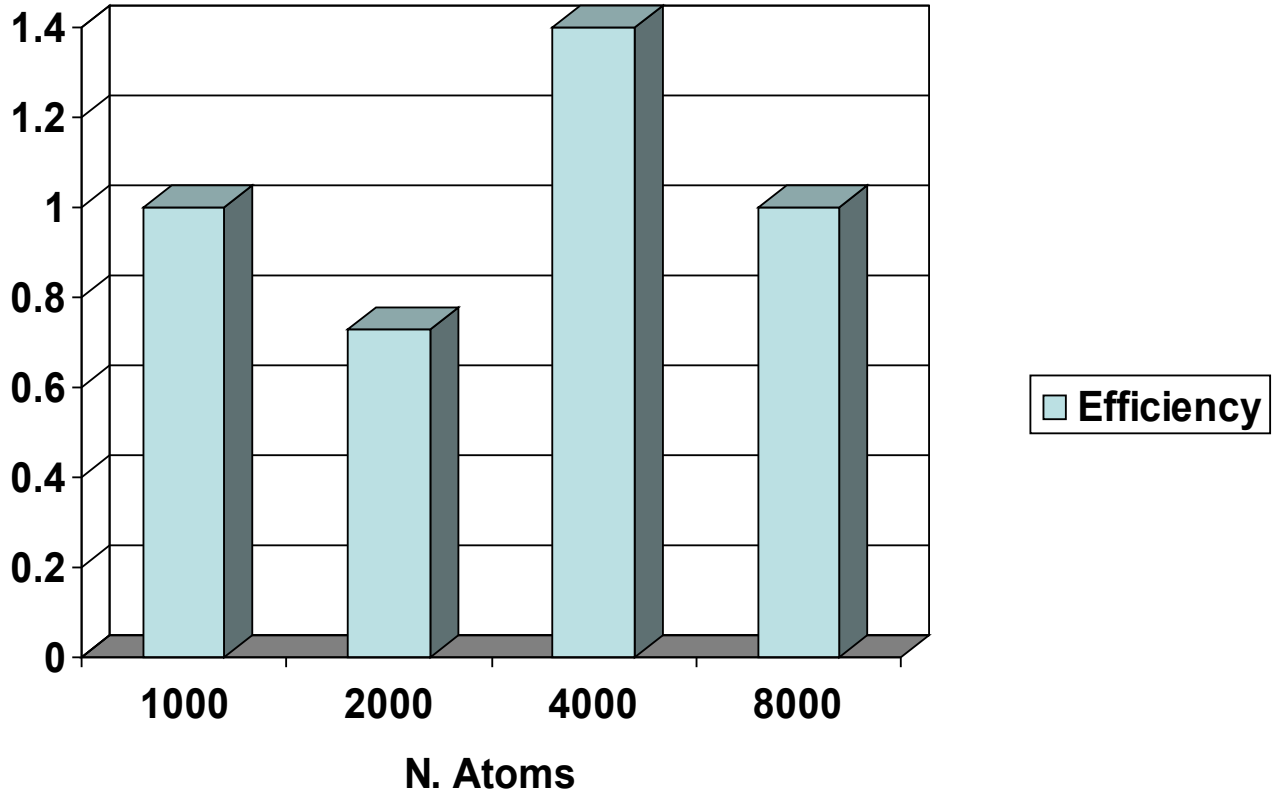




Best Time per step = 12.0 sec (Li_2O_2) - 2.84 sec (PC)

~ 20 ps / week on 2048 proc

Test 3: Ab-Initio Simulations on large systems (Silicon Carbide supercells)



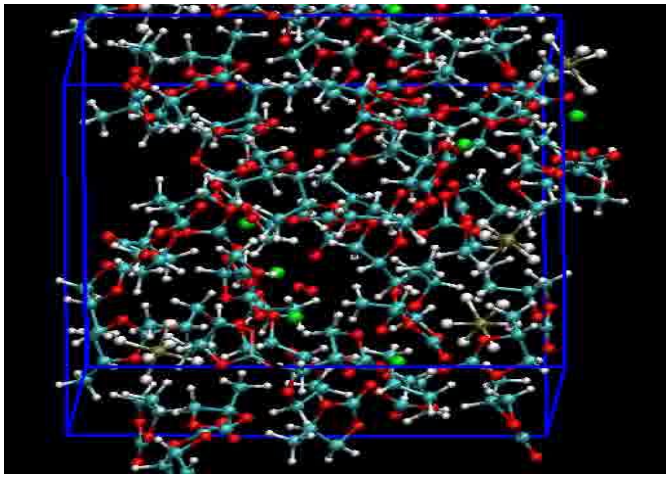
1000 atoms (4000 electrons) 1BG/P Rack time/step : 4 sec BG/P

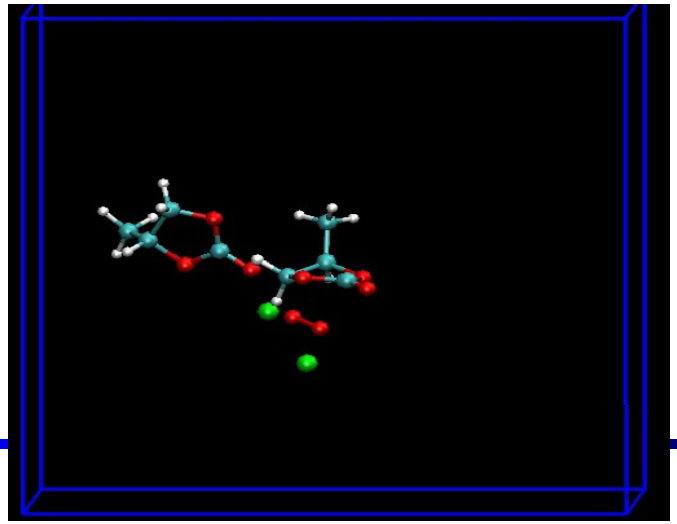
2000 atoms (8000 electrons) 2BG/P Racks time/step : 25 sec BG/P

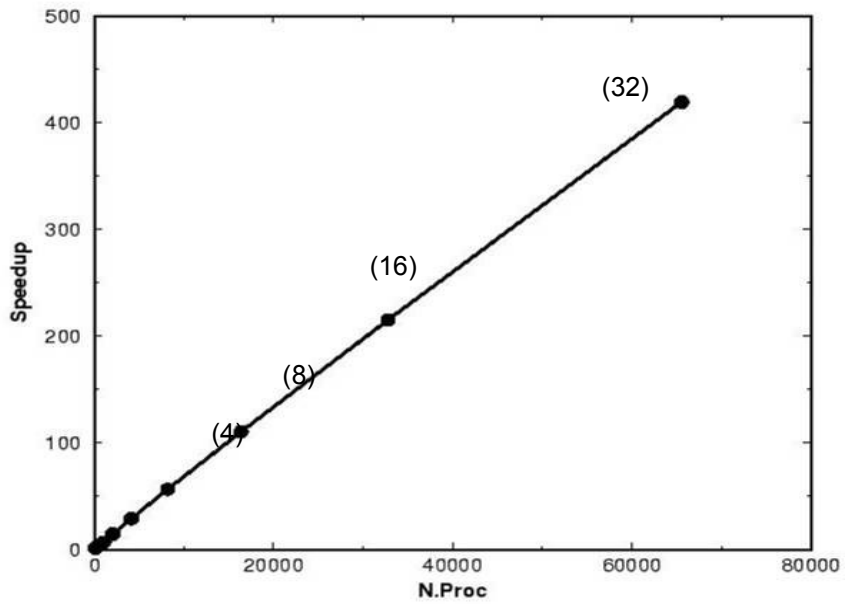
4000 atoms (16000 electrons) 2BG/P Racks time/step: 97 sec BG/P

8000 atoms (32000 electrons) 4BG/P Racks time/step: 540 sec BG/P

Test 4: Exploiting Intrinsic Parallelism: Multiwalker Metadynamics



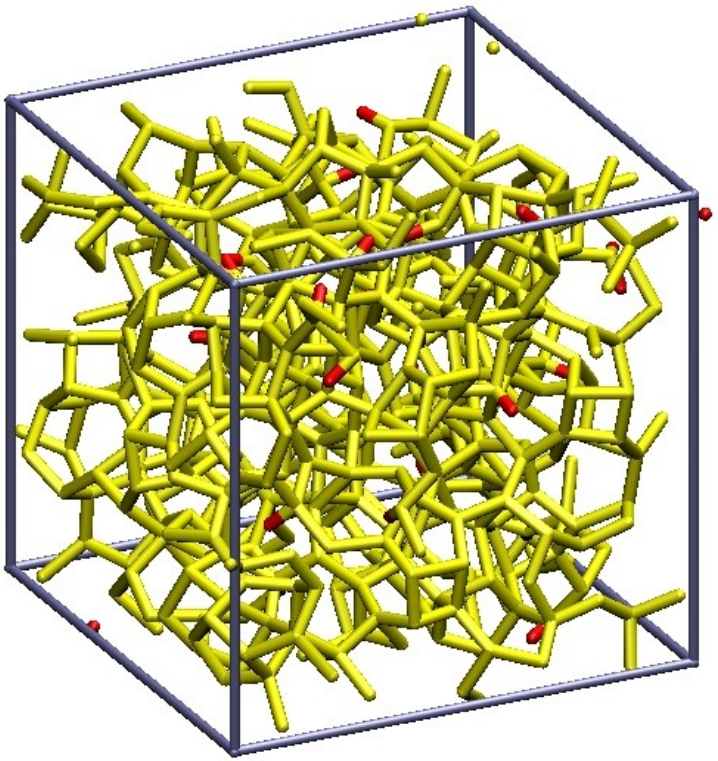


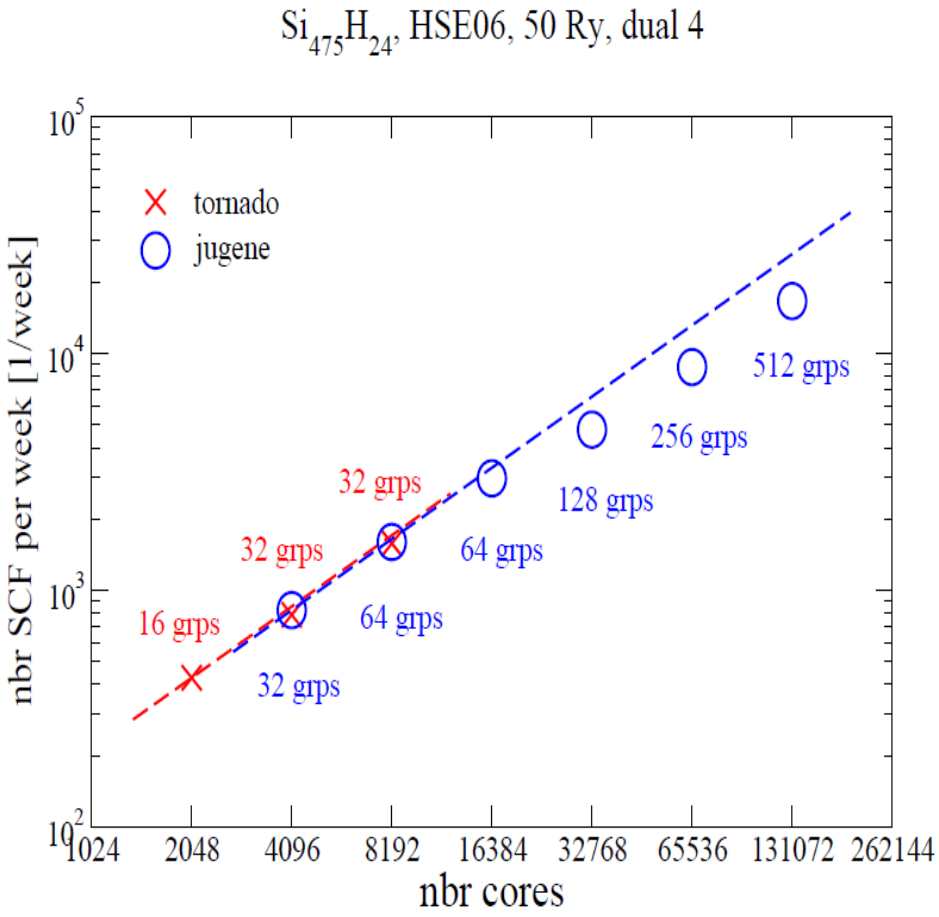


Aprotic Solvent Stability in Li-air batteries
Propylen Carbonate + LiPF6 +Li2O2
~600 atoms – 300 K
~10ps 1Week → 5hours
Screening Possible!

(runs ANL – scaling Juelich)

Test 5: aSiH - Hybrid Functional





Best Time per step = ~30 sec

Opportunities

- System Sizes: ~1'000'000 atoms ?

- Throughput: ~ 100-1000 ns/week (hundreds atoms)
  1 ns/week (thousand atoms)

- Accuracy (effective meta functionals)

- Accurate Complex Chemistry/Materials Science via Enhanced Sampling (Metadynamics, Path Sampling)

- Possible exploitation of Millions of Threads

Outline of the Presentation

- Introduction
  - Computational Sciences at IBM Zurich Research Laboratory
  - The need of extreme parallelism
- The CPMD code: a research tool for ab-initio MD
  - CPMD parallelization and scaleout
  - Cache/Network Optimized Orthogonalization
  - Performance on tests systems : time scales and system sizes
- The new challenges toward exascale computing
  - Fault tolerant and energy efficient algorithms
- Succesfull application examples
- Conclusions

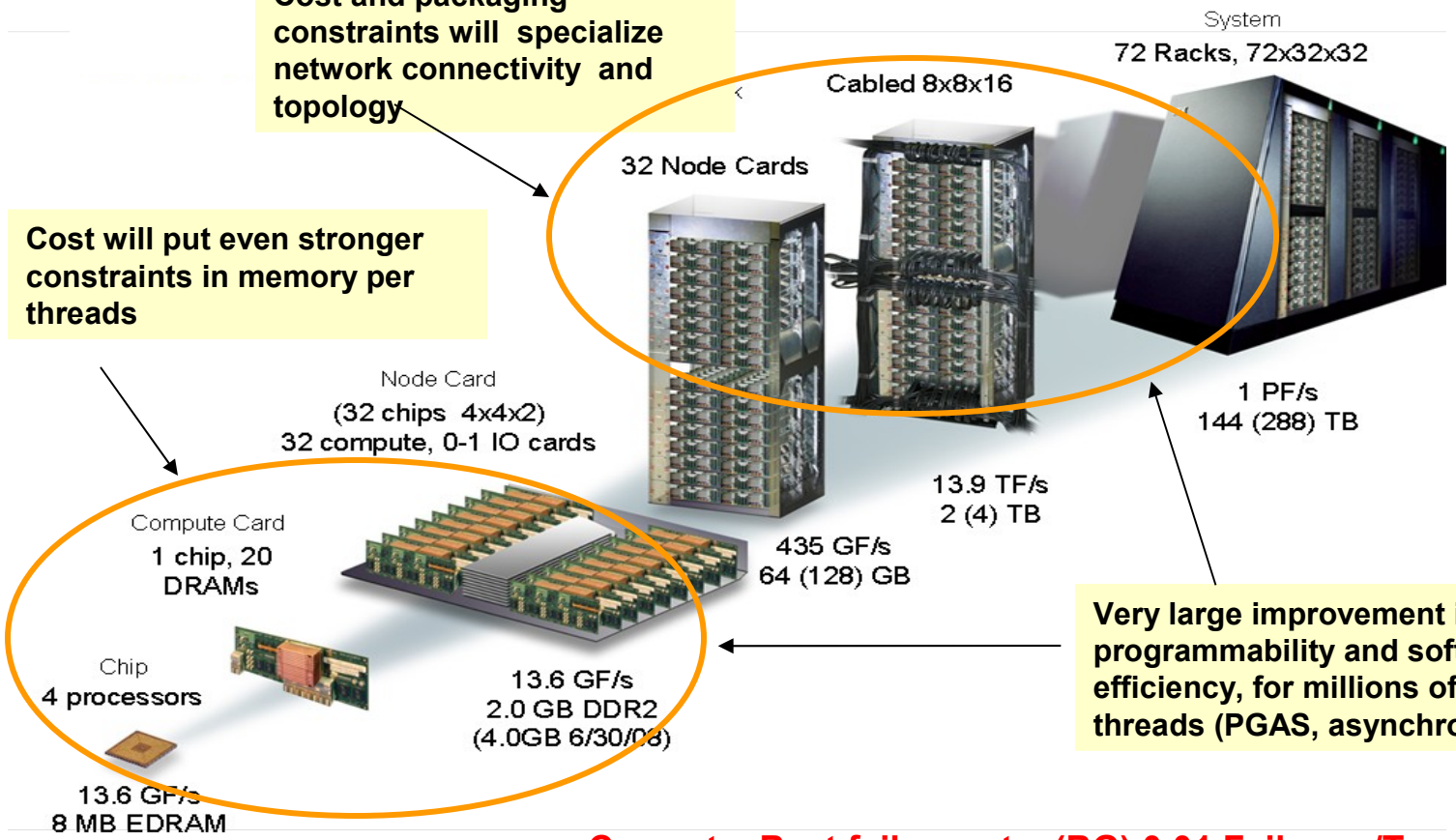
Deep Computing Research:
Exascale: Innovation areas demanded by power, cost and usability
(20MWatts vs 2GWatts)

1000x

Several Millions of computing threads

Cost and packaging constraints will specialize network connectivity and topology

Cost will put even stronger constraints in memory per threads



Very large improvement in programmability and software efficiency, for millions of threads (PGAS, asynchronous)

Current – Best failure rate (BG) 0.01 Failures /Teraflops/Month

1 Failure every 4 Minutes at Exaflop

Energy Efficient and Fault Tolerant Algorithms

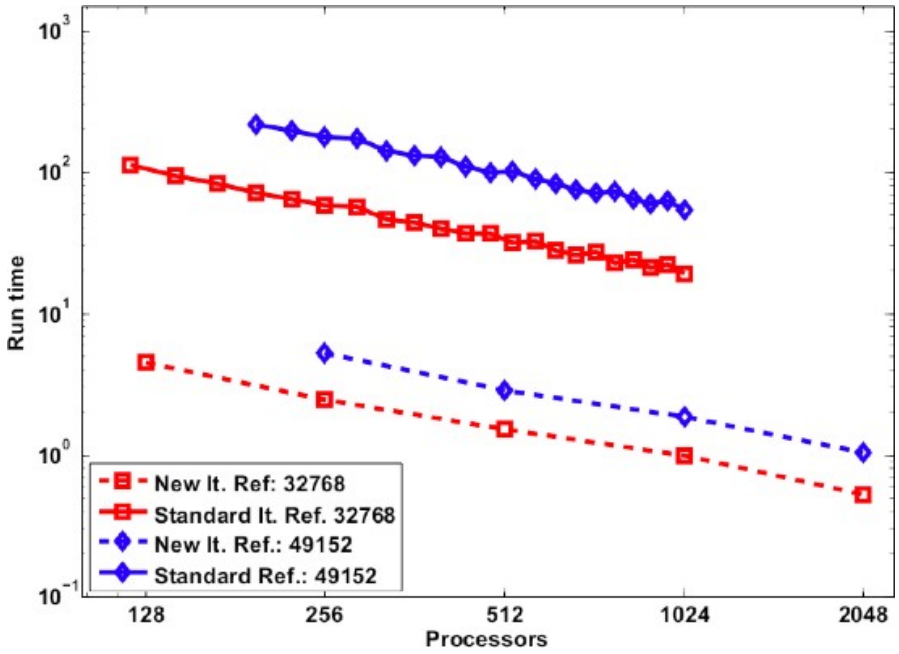
Serial	Multicore/Parallel	Extreme Parallel Heterogeneous	New Concepts	System
Flops/sec	Flops/sec/Watt	TTS*Energy		Metric
Optimized for stustained performance	Optimized for sustained performance & energy	Optimized for TTS, Energy & Fault Tolerance		Algorithm

- Algorithm research will play an increasing role in Exascale computing Research.
- Focus shift from Sustained Performance to Energy Efficiency and Fault Tolerance.

Energy Efficient and Fault Tolerant Algorithms

- Re-engineering of simulation methods and algorithms using time to solution, energy efficiency and fault tolerance as optimization criteria
  - -System constraints : extreme parallelism, low ratio memory/computation, low ratio communication/computation, data locality, (programmable)-accelerators

- Example: Iterative Linear Solver with Mixed Precision (C. Bekas and A. Curioni)



Qadratic Cost Iterative Refinement:
~ 1 sec time to solution
~ 12 % sustained performance
~ 0.005 kWh energy usage
Fault Tolerant (~10% cost)

Standard Iterative Solver:
~20 sec time to solution
~9 % sustained performance
~0.0116 kWh energy usage
Fault Tolerant(~10% cost)

Standard Direct Solver (Linpack):
~15 sec time to solution
~80% sustained performance
~0.0441 kWh energy usage
Non Fault Tolerant (~100% cost)

Quadratic Cost Iterative Refinement

- ✓ LOW PRECISION: LP
- ✓ HIGH PRECISION: HP
- ✓ Let CG(A,y,k) be a procedure implementing k steps of Conj. Gradient in single precision

1. Compute initial solution: x_0=CG(A,b,k) Cost: $O(kn^2)$
2. Compute initial residual: $r_0 = b - Ax_0$ Cost: $O(n^2)$
3. k = 0
4. REPEAT
   6. Solve for residual: d_k= CG(A,r_k,k) Cost: $O(kn^2)$
   7. Update solution: $x_{k+1} = x_k + d_k$ Cost: O(n)
   8. Compute residual: $r_{k+1} = b - Ax_{k+1}$ Cost: $O(n^2)$
   9. k = k + 1
10. UNTIL $||r_{k+1}|| \cdot tol$

Key properties:

- ✓ **Dominant cost $O(kn^2)$. Performed in LOW PRECISION**. Cost in HP is $O(n^2)$
- ✓ We can take great advantage of fast single precision hardware!
- ✓ Even on platforms without fast low prec hardware: benefit (30% or so) from reduced memory traffic

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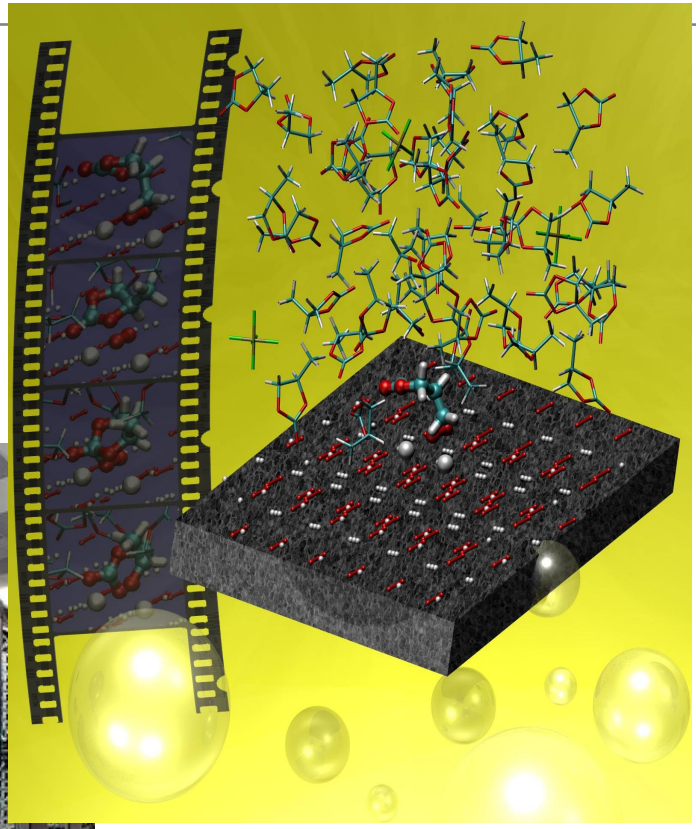
- Conclusions

BAT500 - HPC based Simulations and Computer Aided Design

Unveiling new pieces in the puzzle of Lithium-air-batteries

- **Activities and Results**
  - electronic bandstructures of Li_xO_y → conductivity
  - overvoltages – or lack thereof
  - **extensive study and forecasts of electrolyte solvent stability**
  - electron transport in Li_2O_2
- **Mostly done on a very large IBM Blue Gene at DOE Argonne National Lab**
  - by the Computational Sciences team at IBM Research – Zurich
  - Recipient of INCITE multiple INCITE awards
  - Instrumental to close collaboration with external partners

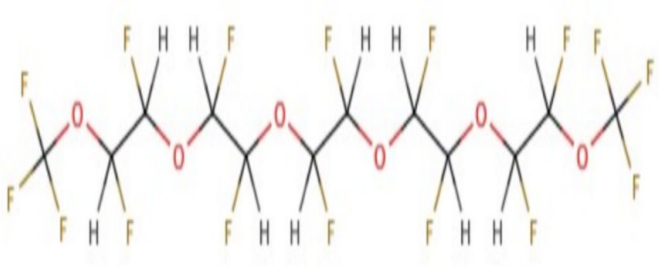


Simulations of Li_2O_2 in Propylenecarbonate, T. Laino, A. Curioni, A New Piece in the Puzzle of Lithium/Air Batteries, Chemistry, DOI 10.1002/chem.201103057 (22 February 2012)

Blue Gene/P at Argonne National Lab (Source: Argonne NL)

Lithium/Air Batteries: screening new solvents

- **Suggest a new class of solvents with strong chemical resilience to Li_2O_2 degradation.**

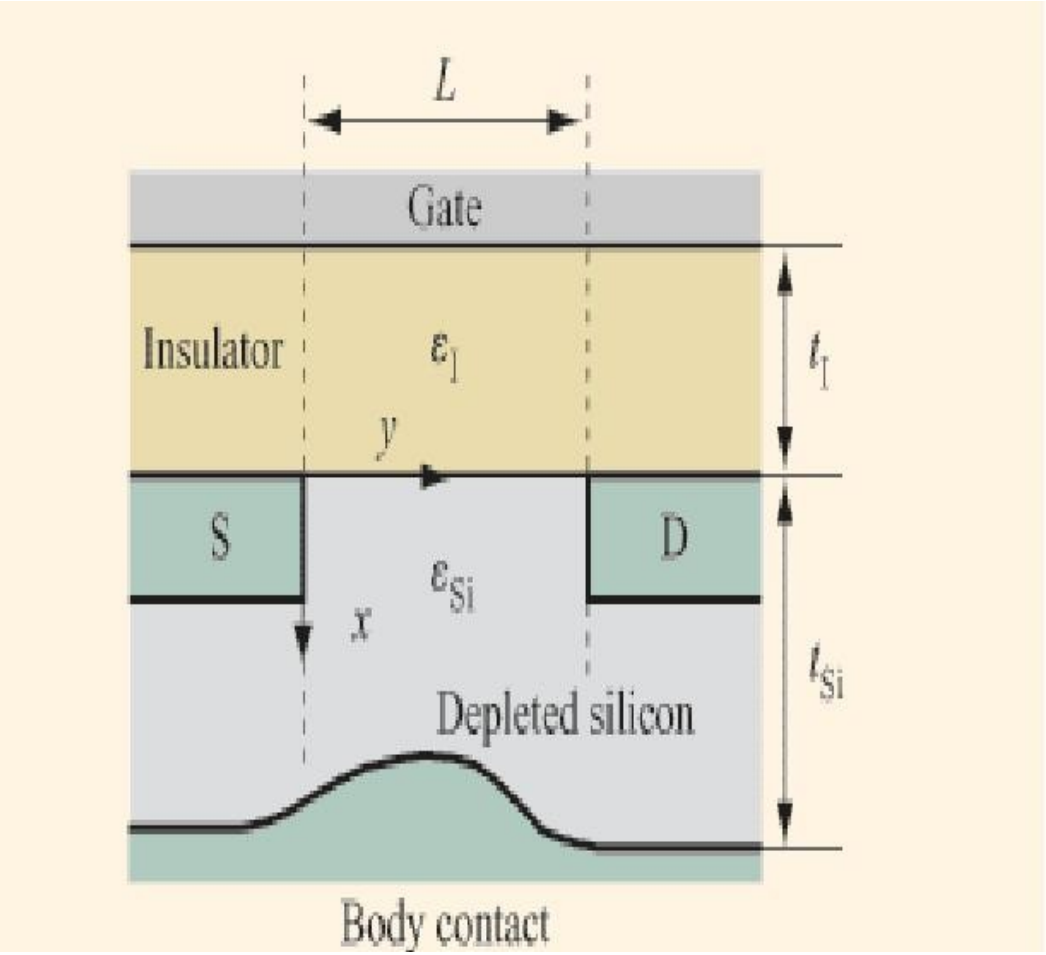


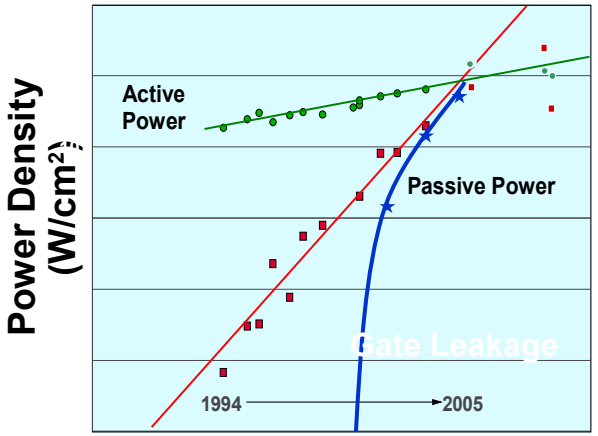
Solvent	Energy Barrier (kcal/mol)
PC	– (*)
NMP	24
NMP-tBut	33
NMP-F3	– (*)
NMP-F6	– (*)
2Met-NMP	51
PEG-5	16
Met-PEG-5	23
F-PEG-5	40
CH3CN	35

(*) spontaneously decompose

Supercomputing for Energy: Batt500 project

Example : IBM Technology – CMOS - Scaling





Gate Length (microns)

Dielectric constant: ε ~ 10 - 40,
Band gap > 6 eV
Non-reactive with Si .
Small electrical thickness (<1 nm);(εSiO2/ε)t
Electrical properties ~ Si/SiO**2**
(low interface defect density, high electron mobilities, low charge trapping)

Computer aided design of materials with tailored properties

Need to calculate structural, electronic and dielectric properties of many candidate materials on realistic environments.
(system sizes ~1000 atoms)

BG/P, allowing to simulate more complex systems for longer timescales, makes computer aided materials design a reality.

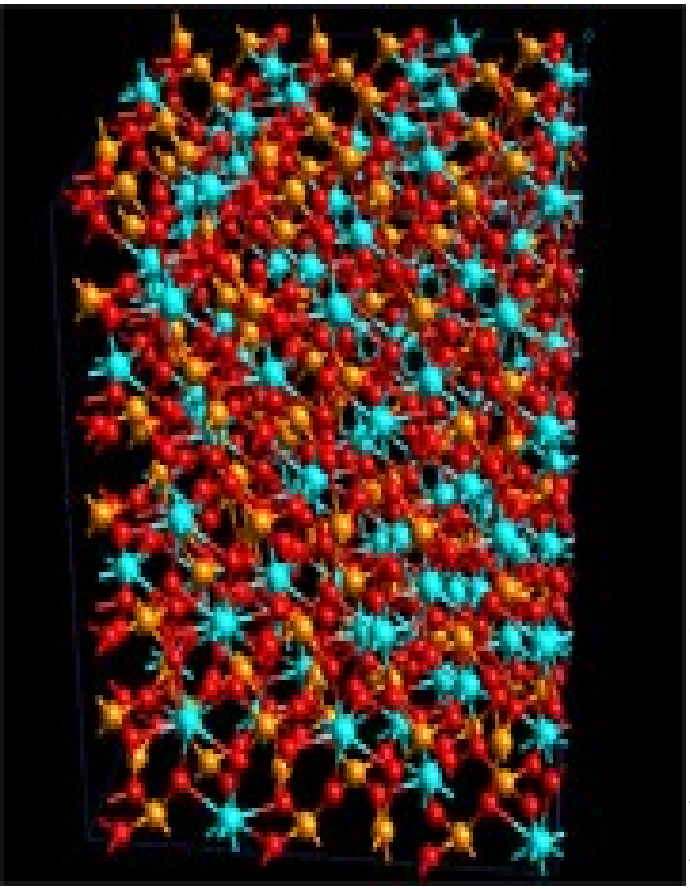
~20.000 Atoms from First Principles based Molecular Dynamics –

20 Millions Atoms per BG/P rack with Classical (Empirical) Molecular Dynamics

$Hf_xSi_{1-x}O_2$: Gate materials optimization

"Odd" observed behavior explained !

C. Pignedoli, A. Curioni, W. Andreoni PRL 98, 037602 (2007)



- First Principles Calculations of structures, chemical/physical stability, electronic and electrical properties (dielectric constants) as a function of Hafnium concentration.

- More then 50 virtual samples of Hafnium silicates were simulated in our in-silico study.

- Blue Gene, its scalability and flexibility plus the optimal remapping of our algorithms have been instrumental for the success of our study.

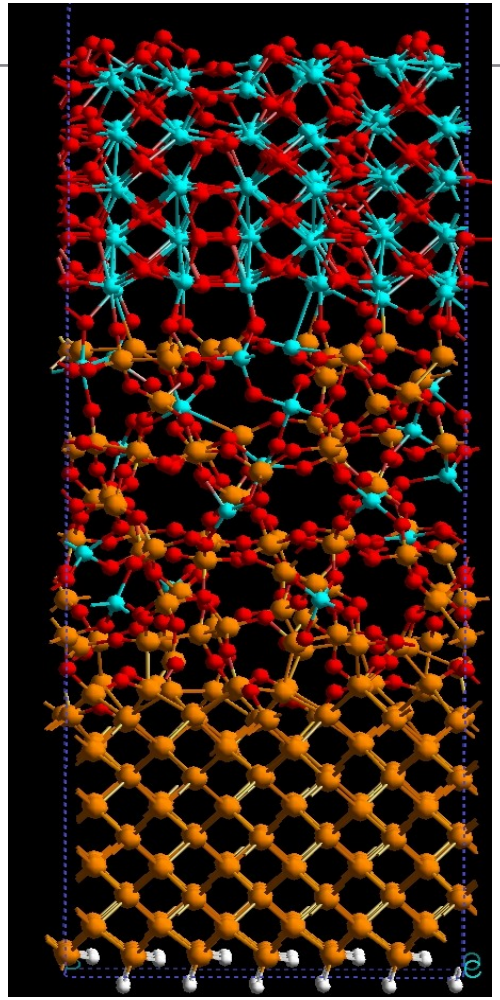
- A single simulation took ~ 5 days on 2 BG/L racks- it would have taken more then 3 months on 8 Racks p690 with Federation switch.

2006 'Interface Engineering for Enhanced Electron Mobilities in W/HfO2 Gate' Stacks' (US7115959)'

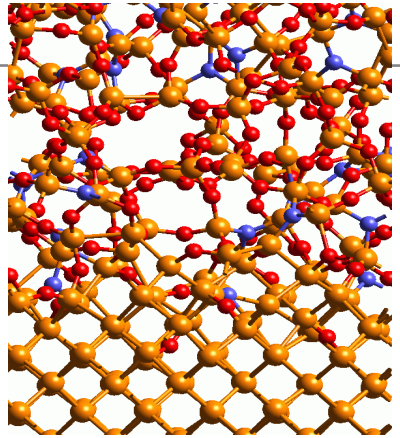
High-K materials

Understand/Develop:

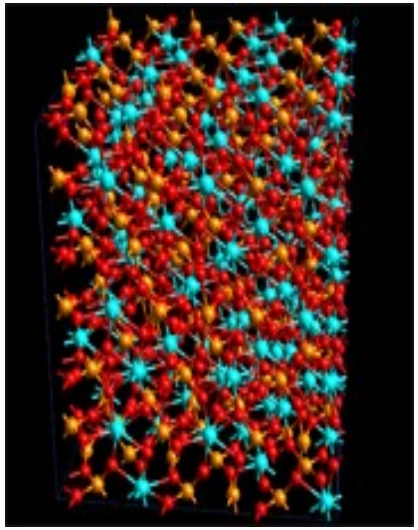
- Structure of the Si/SiO2/HighK interface
- Dependence of the K on chemical composition in SiOxNy
- Odd behavior of the K in Hf/Zr Silicates
- Accurate model for vacancy diffusion in LaxHfyOz systems
- issues of integration of Ultra-High-K materials



Si/SiO2/HfO2 stack



SiON/SiO2 interface



Hafnium Silicate

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THANK YOU!