Optimizing Large Scale Chemical Transport Models for Multicore Platforms

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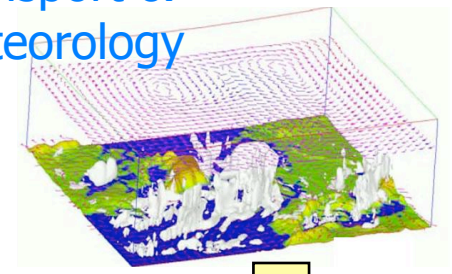
Introduction: How do we apply new technology to existing algorithms? Pros? Cons?

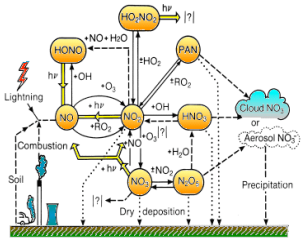
- Modern hardware is parallel, becoming massively parallel, becoming **hetero**geneous
- Parallel hardware is increasingly diverse
  - Shared and distributed memory in the same system
  - Homo-/Heterogeneous clusters of Homo-/Heterogeneous hardware
- Air quality models are computationally-intense multi-scale multi-physics models
  - Computationally-intense → motivates parallelism
  - Multi-scale → leverages a wide range of algorithms
  - Multi-physics → leverages a wide range of technologies

Comprehensive AQMs motivate parallelization

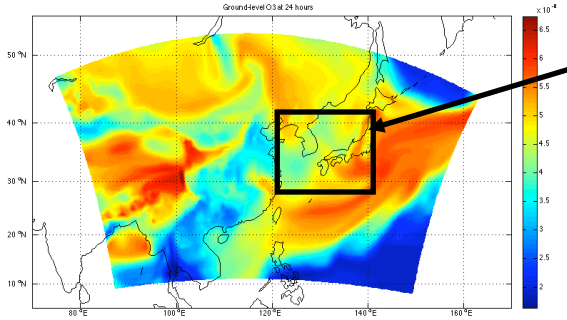
Transport & Meteorology

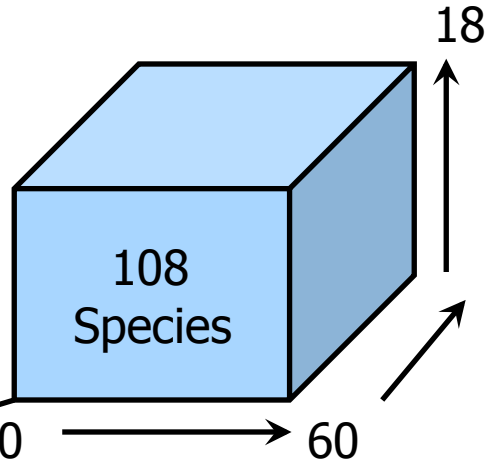


Chemical kinetics

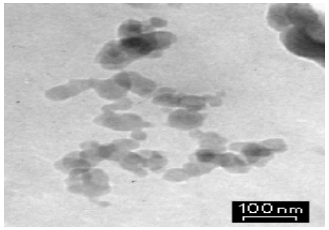


STEM





Aerosols



Emissions

90 x 60 x 18 x 108 =
10,497,600 variables

(10,497,600 x 64) / 8 =
~80MB per iteration

Mass-balance equations for trace species determine the fate of pollutants in the atmosphere

Boundary $\partial\Omega = \Gamma^I \cup \Gamma^o \cup \Gamma^G$

1a. $$\frac{\partial c_i}{\partial t} = -u \cdot \nabla c_i + \frac{1}{\rho}\nabla \cdot (\rho K \nabla c_i) + \frac{1}{\rho} f_i(\rho c) + E_i$$

1b. $$c_i(t^0, x) = c_i^0(x)$$

1c. $$c_i(t, x) = c_i^I(t, x),\ x \in \Gamma^I$$

1d. $$K\frac{\partial c_i}{\partial n} = 0,\ x \in \Gamma^O$$

1e. $$K\frac{\partial c_i}{\partial n} = V_i^{dep} c_i - Q_i,\ x \in \Gamma^G,\ \text{for all } 1 \le i \le s.$$

These equations are solved in a sequence of N time steps of length Δt taken between t^0 and $t^N = T$. *[Sandu et al., 2005]*

Mass-balance equations for trace species determine the fate of pollutants in the atmosphere

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1d. $$K\frac{\partial c_i}{\partial n} = 0,\ x \in \Gamma^O$$

1e. $$K\frac{\partial c_i}{\partial n} = V_i^{dep} c_i - Q_i,\ x \in \Gamma^G,\ \text{for all } 1 \le i \le s.$$

Transport
u: wind vector field
ρ: air density
K: turbulent diffusivity tensor

These equations are solved in a sequence of N time steps of length Δt taken between t^0 and $t^N = T$. *[Sandu et al., 2005]*

Mass-balance equations for trace species determine the fate of pollutants in the atmosphere

Boundary $\partial\Omega = \Gamma^I \cup \Gamma^o \cup \Gamma^G$

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Chemistry
f_i: transformation rate

These equations are solved in a sequence of N time steps of length Δt taken between t^0 and $t^N = T$. *[Sandu et al., 2005]*

Mass-balance equations for trace species determine the fate of pollutants in the atmosphere

Boundary $\partial\Omega = \Gamma^I \cup \Gamma^o \cup \Gamma^G$

1a. $$\frac{\partial c_i}{\partial t} = -u \cdot \nabla c_i + \frac{1}{\rho}\nabla \cdot (\rho K \nabla c_i) + \frac{1}{\rho} f_i(\rho c) + E_i$$

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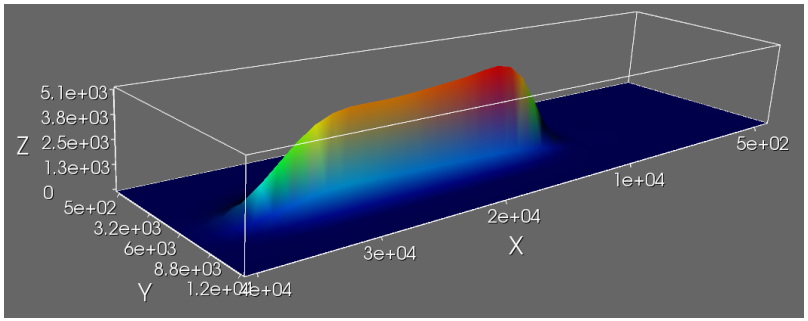
1e. $$K\frac{\partial c_i}{\partial n} = V_i^{dep} c_i - Q_i,\ x \in \Gamma^G,\ \text{for all } 1 \le i \le s.$$

Above-Ground Emissions

These equations are solved in a sequence of N time steps of length Δt taken between t^0 and $t^N = T$. *[Sandu et al., 2005]*

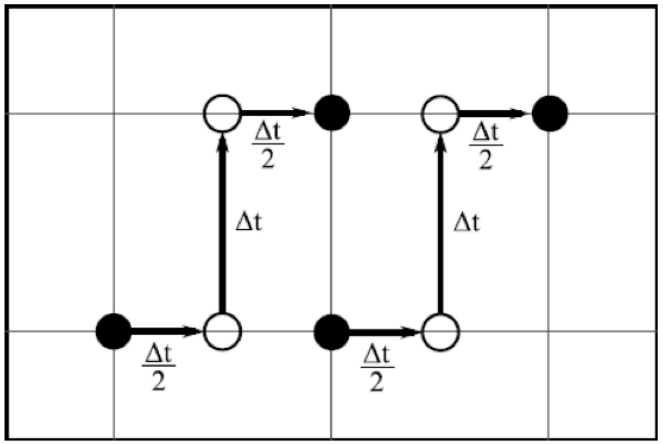
FIXEDGRID is a prototype AQM for multicore Systems

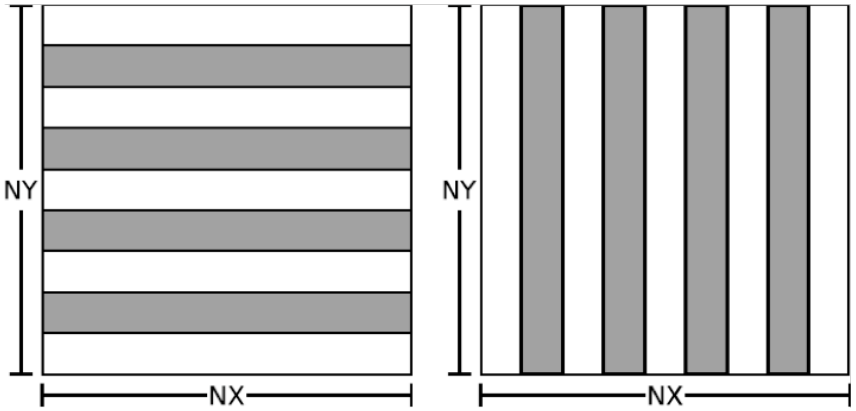
- Simplified multi-scale atmospheric model
- Explicit time-stepping in transportation
- SAPRC'99 chemical mechanism
  - 79 species, 211 reactions, stiff system
- Research code to easily compare a range of computing platforms
- Written in Fortran 90



FIXEDGRID uses dimension splitting to simplify computation and reduce round-off error

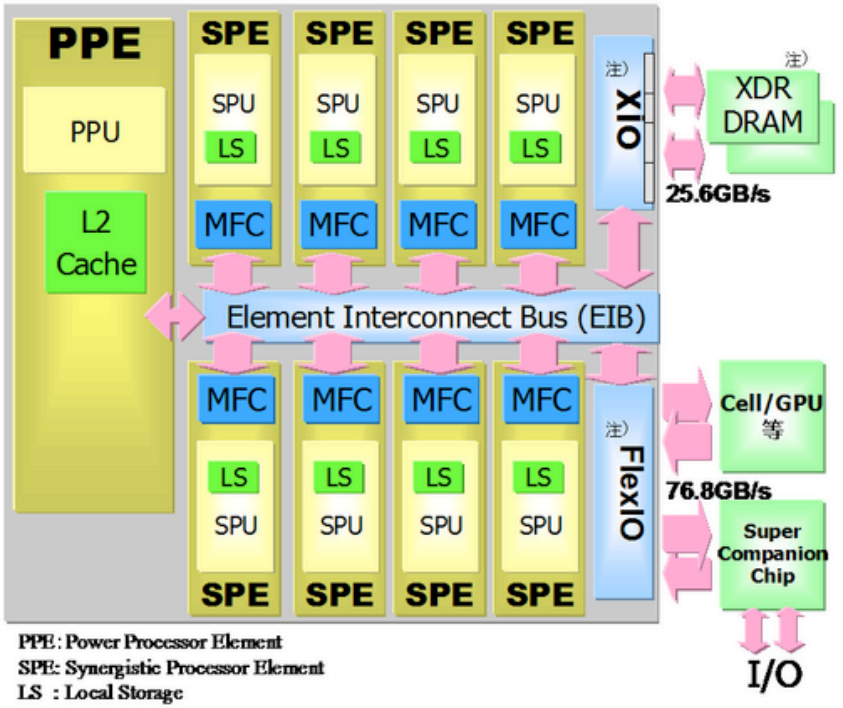
- X / Y dimension spliting reduces program complexity
- Rows / Columns explicitly discretized and solved with the same code routine
- Symmetric 2nd order time-dimension spliting reduces round-off error





The Cell Broadband Engine is a heterogeneous CMP

- 1 Power Processor Element
  - 64-bit, dual threaded
  - Vector/SIMD extensions
- 8 Synergistic Processor Elements
  - 128-bit, single threaded
  - Vector/SIMD extensions
  - 128 128-bit registers
  - 256KB local storage
  - Optimized for 32-bit **single-precision** floating point
  - Memory Flow Controller supplies asynchronous DMA
- 204.8GB Peak EIB Bandwidth



The Cell memory model has “interesting features”

- SPEs must use DMA to access main memory
  - Data must be “correctly” aligned
  - Minimum transfer size is 16 bytes
  - Data must be contiguous
  - Data should be 128-byte aligned
- SPEs have only 256K of local storage (~8,000 doubles)
- PS3 reserves two SPEs
- PS3 has less memory than CBE blade

We produced four versions of FIXEDGRID

1. Translated Fortran to C
2. Moved computational cores to the SPEs
3. Optimized SPE code
4. Implemented scalable strided main-memory access method

	Ver. 1	Ver. 2	Ver. 3	Ver. 4
0	2638			
1		3965.45	1271.25	1118.95
2		2095.02	771.30	632.94
3		1430.63	678.99	490.58
4		1137.48	658.42	423.19
5		988.32	643.89	389.89
6		928.20	646.30	375.96

Runtime in seconds for 1000 x 700 grid points

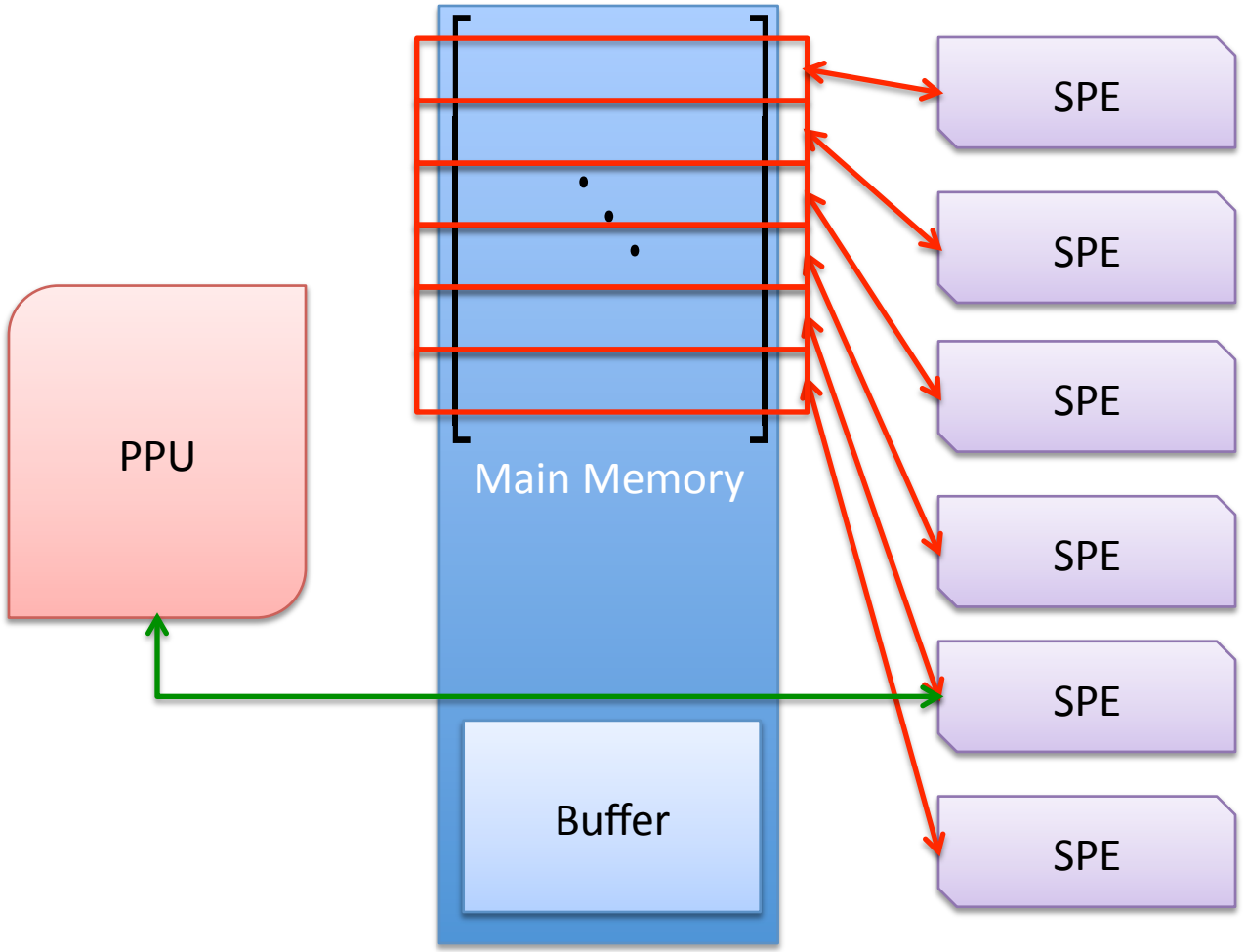
FIXEDGRID Version 1: Baseline

- No Fortran compiler in CBE SDK 2.2
  - SDK 3.0 includes a modified version of XL Fortran
- Automatic Fortran → C translation is available, (i.e. f2c) but we did it by hand
  - Improve source code readability
  - Refactor code to better fit the execution model
- Translation "rules of thumb:"
  - `parameter` → `#define`
  - `using module` → `#include`
  - Fortran array syntax → C macros (when possible)
- Long, tedious, bug-prone, not recommended for real-world codes (approx. 38 work hours, ~2,000 lines)

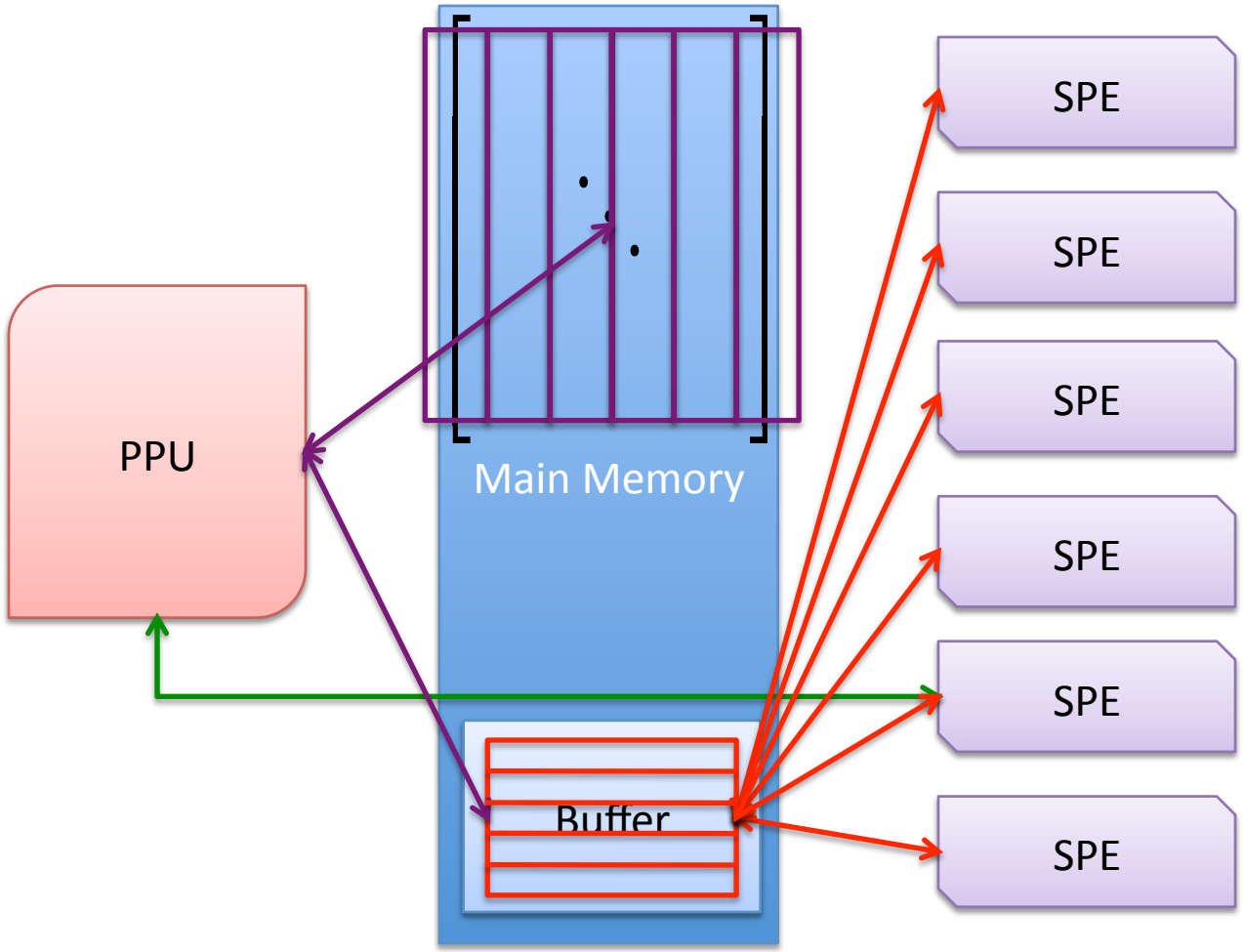
FIXEDGRID Version 2: Parallelized baseline

- Offloaded the main computational cores: `discretize()` and `advec_diff()`
- Implemented generic data types for passing arguments to the SPUs
- Implemented tiny 32-bit communication library for PPU / SPU communication
  - Send/receive to/from SPUs
  - Broadcast to SPUs
  - Synchronize PPU with one/all SPUs

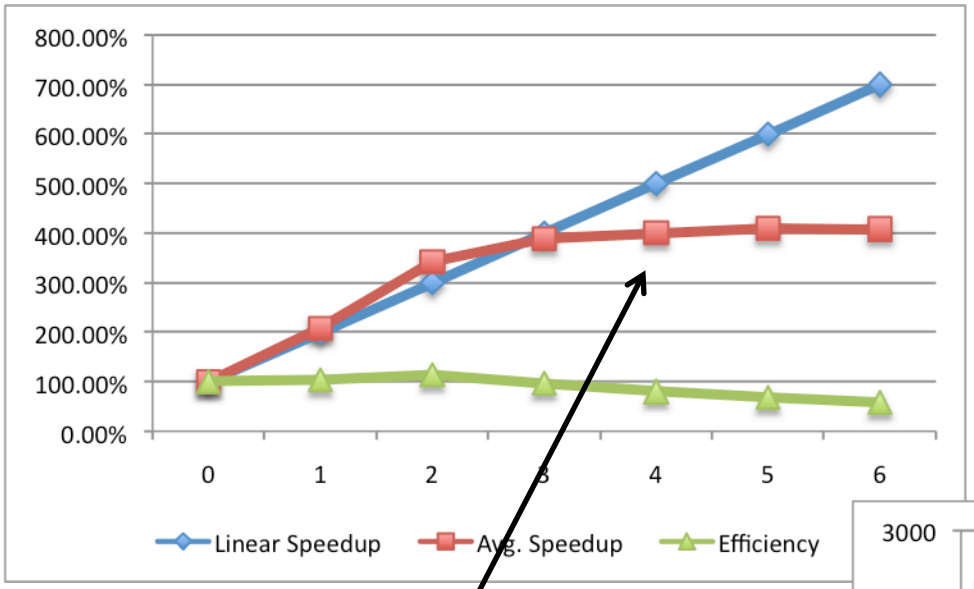
SPEs copy matrix rows directly from main memory



PPU buffers transposed columns in main memory

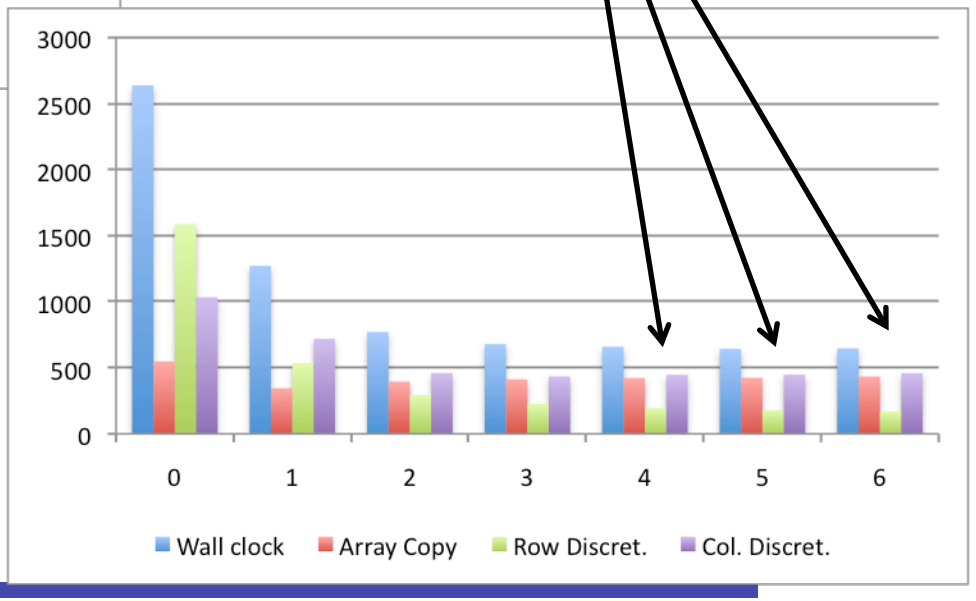


Reordering matrix column data is a severe bottleneck



Scalability limited by memory bottleneck

Column discretization bounded by array copy



FIXEDGRID Version 3: Optimized SPU code

Optimization	Runtime Reduction
Double-buffered DMA	23%
Vectorization and SPU intrinsics	18%
Loop unrolling and branch prediction	8%

Mem[0, BSIZE) → Buffer[0]

Mem [BSIZE, 2*BSIZE) → Buffer[1]

for i in 0, 1, 2, … MATRIX_SIZE / BSIZE

b = i mod 2

Process Buffer[b]

Buffer[b] → Mem[i*BSIZE, (i+1)*BSIZE)

Mem[(i+2)*BSIZE, (i+3)*BSIZE) → Buffer[b]

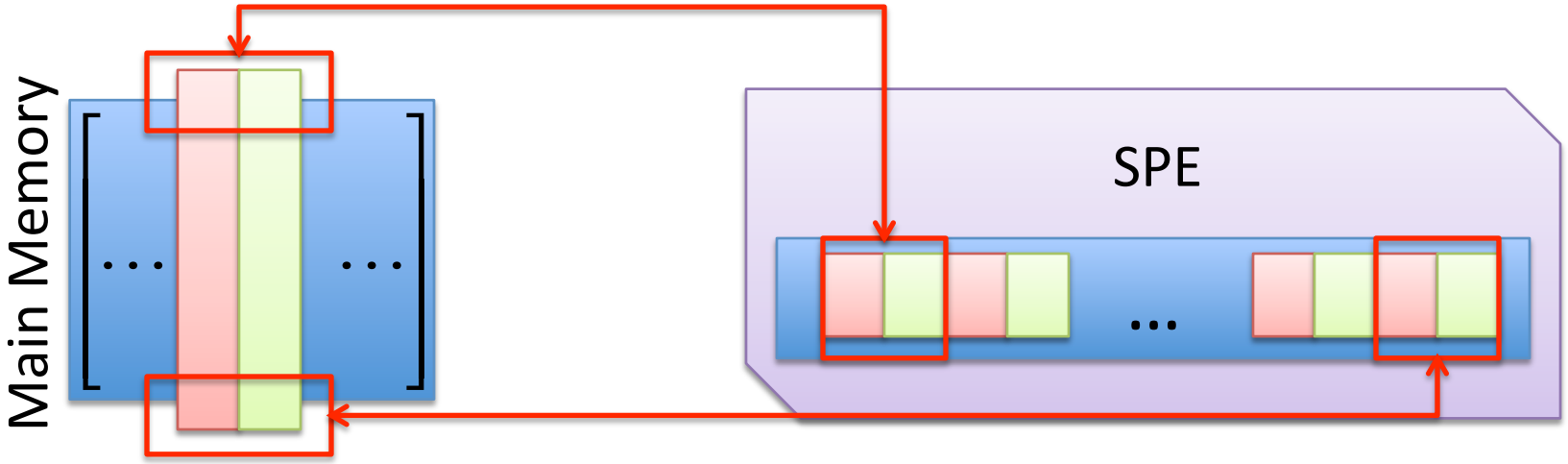
end

Fetch, process and write any remaining buffer

```
vector double sum_d;
vector double vec1_d =
    {buff[i], buff[i+1]};
vector double vec2_d =
    {buff[i+2], buff[i+3]};
sum_d = spu_add(vec1_d, vec2_d);
```

FIXEDGRID Version 4: Scalable non-contiguous DMA

- Use DMA lists to reduce overhead for multiple consecutive transfers
- Minimum transfer size is 16 bytes, so transfer two double precision variables
- Columns arrived interleaved into SPE local storage

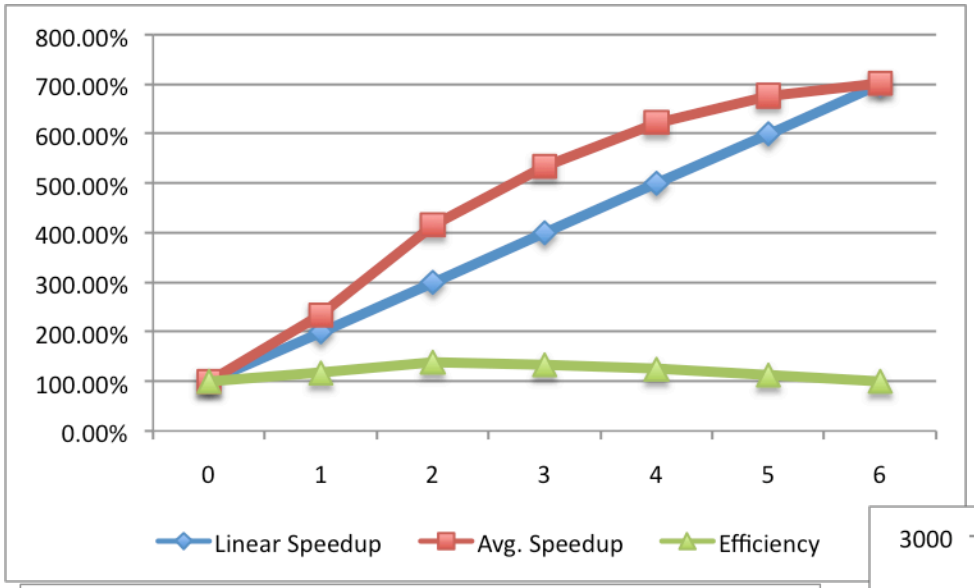


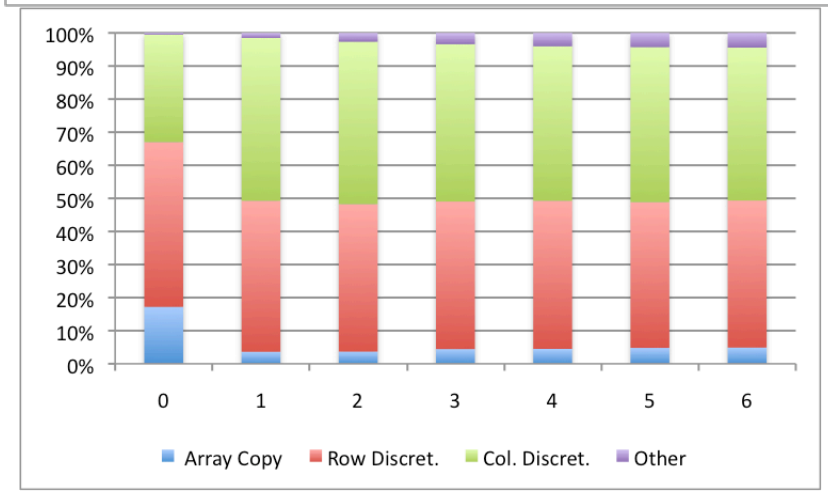
Scalable strided DMA requires O(n) overhead storage

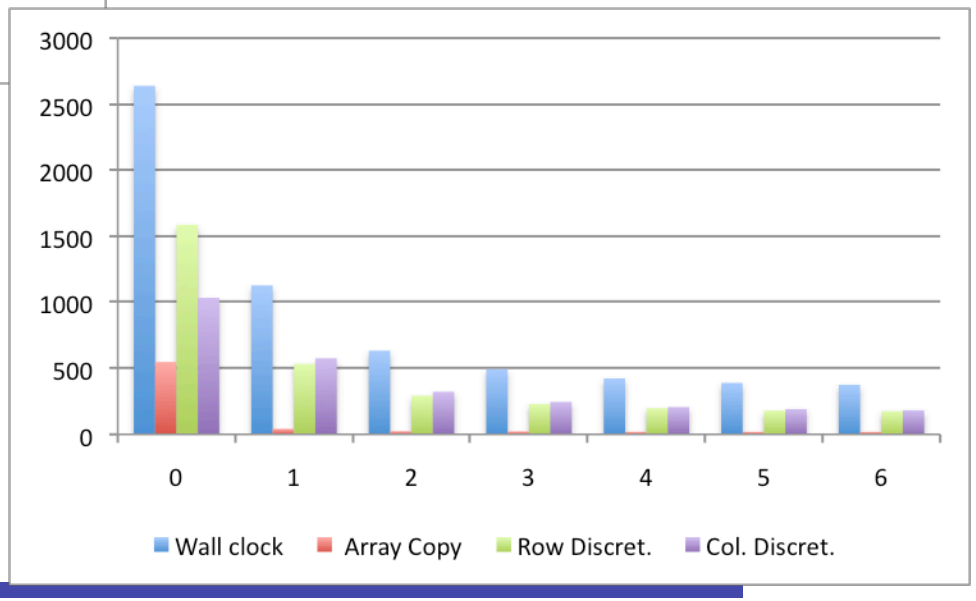
- DMA lists reside in SPE local storage
- List of pairs of 64-bit address lower bits and transfer lengths
- One DMA list element is required for each 16 byte transfer

```
typedef struct {
  union {
    unsigned int all 32;
    struct {
      unsigned nbytes: 31;
      unsigned stall:   1;
    } bits;
  } size;
  unsigned int ea_low;
} dma_list_elem_t;
```

FIXEDGRID performs exceptionally well on the Cell



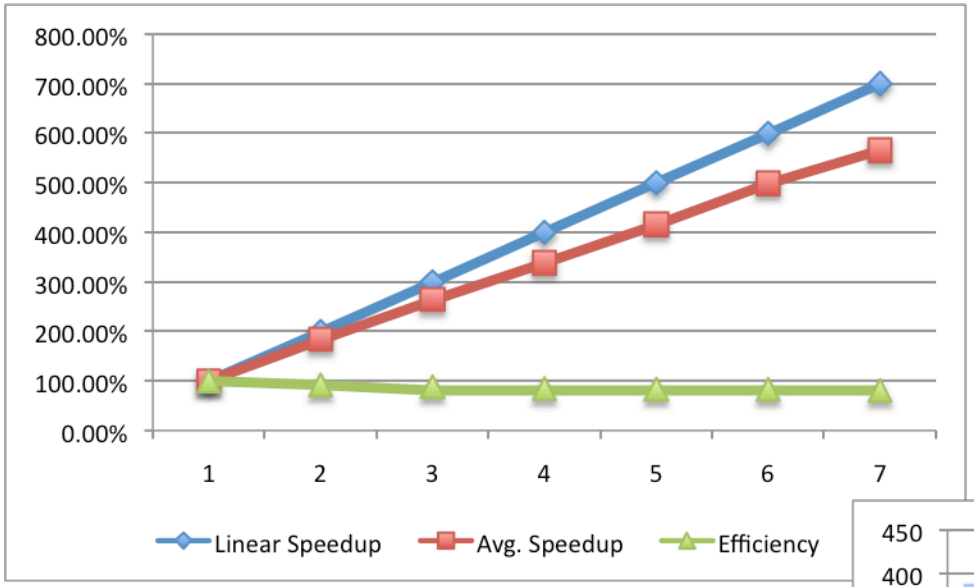


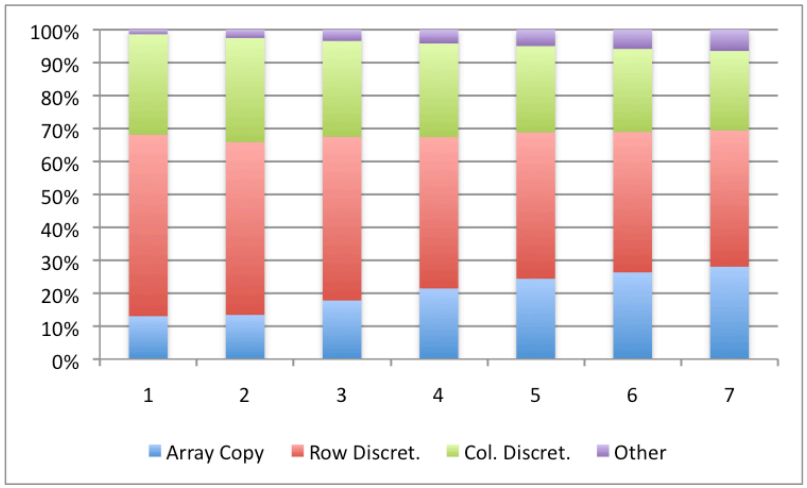


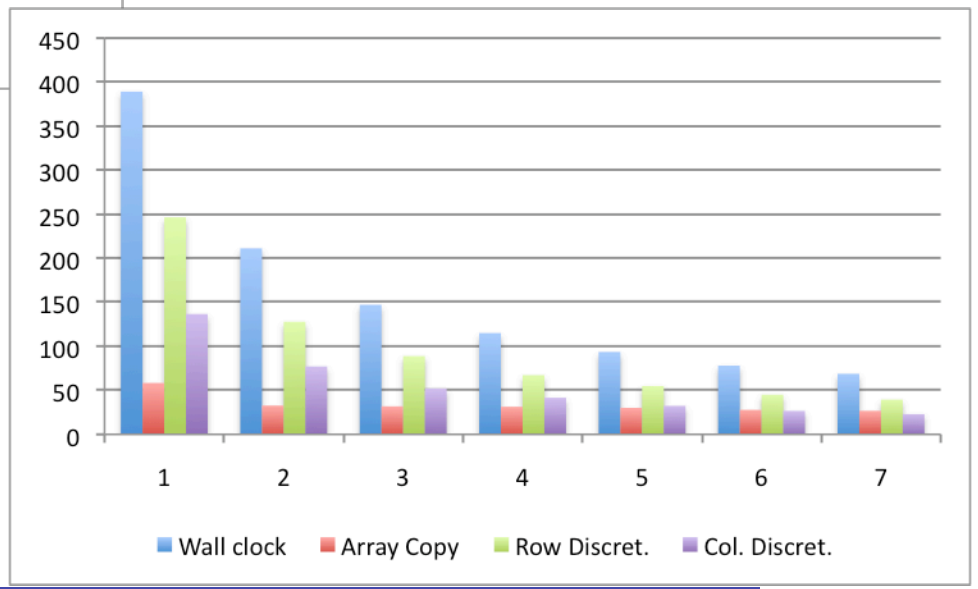
We parallelized FIXEDGRID Version 1 with OpenMP

- Trivial to implement, less than 4 hours, ~50 lines of code
- Test platform: dual Intel Quad-Core Xeon shared-memory workstation

FIXEDGRID scales well on a homogeneous system







Conclusions

- Heterogeneous accelerated CMPs can significantly improve the performance of large-scale chemical transport models
- Porting a small Fortran code to CBE was non-trivial. Porting larger codes would be impractically difficult without better tools.
- Hardware support for non-contiguous memory access in CBE should be considered.
- Alternate matrix storage formats should be considered for accelerated CMPs with limited main-memory access from accelerators

Thank you