Computing Turbulence in the $4096^3$ Range

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Collaboration with

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Outline of Talk

I) Overview of DNS on the Earth Simulator and VPP

II) Visualization

III) Some DNS Results
I) Overview of DNS on the Earth Simulator and VPP
Computational Facilities & Performance

★ 1 (512³) & ★ 2 (1024³)
- Fujitsu vpp500/42, VPP5000/56 (Nagoya UCC)
  0.5TFLOPS (peak), Memory 0.9TB

★ 3 (2048³) & ★ 4 (4096³)
- Earth Simulator (2002)
  40TFlops (peak), 16.4TFlops (sustained),
  Memory: 10TB
History of representative DNS
Incompressible Homogeneous Isotropic Turbulence under periodic BC

- Orszag (1969): IBM Model 360-95
- Kerr (1985): Cray-1S NCAR
- Siggia (1981): Cray-1 NCAR
- Jimenez et al. (1993): Caltech Delta machine
- Yamamoto (1994): NWT: Gordon Bell Prize
- Siggia (1981): Cray-1 NCAR
- VPP
- VPP5000/56 NUCC (2001)
- I&K, Gotoh & Fukayama
- Yamamoto (1994): NWT: Gordon Bell Prize
- 240^3
- 128^3
- 64^3
- 32^3
- 1024^3
- 2048^3, 4096^3

Number of grid points
16.4 Tflops Direct Numerical Simulation of Turbulence by a Fourier Spectral Method on the Earth Simulator

Mitsuo Yokokawa
Ken’ichi Itakura, Atsuya Uno
Takashi Ishihara and Yukio Kaneda

See: Yokokawa, Itakura, Uno, Ishihara & Kaneda (SC2002)[YIUYK(SC2002)]
http://www.sc-conference.org/sc2002/
& also http://www.ultrasim.info

The slides (No.8-19) are made from this presentation
The Earth Simulator

- **35.86 Tflops** sustained in Linpack benchmark was achieved.
- It’s actually the world fastest supercomputer.
- “TIME” chose it as one of 2002 world inventions.
Configuration of the Earth Simulator

- Total number of PNs: 640
- Peak performance/AP: 8Gflops
- Peak performance/PN: 64Gflops
- Shared memory/PN: 16GB
- Total peak performance: 40Tflops
- Total main memory: 10TB
Features of the Earth Simulator

- One chip vector processor of 8 Gflops
  - 0.15 μm CMOS LSI technology with Cu wiring
  - Large size LSI of 20.79mm x 20.79mm
  - Vector pipeline units at 1GHz and other parts at 500MHz

- SMP cluster
  - High bandwidth memory access of 256 GB/s

- High-bandwidth and non-blocking interconnection crossbar network
  - Aggregate switching capacity of 7.8 TB/s
Overview of DNS code

- Forced incompressible Navier-Stokes equations under periodic BCs.

\[ \frac{\partial u}{\partial t} = u \times \omega - \nabla \Pi + \nu \Delta u + f \]  
(Rotational form) \[ \nabla \cdot u = 0 \]

- Fourier spectral method
- Alias error removed by mode truncation & phase shift
- Fourth-order Runge-Kutta method for time advancing
Implementation of DNS code

- written in Fortran90.

- Eighteen 3D-FFTs are required for evaluations of the right hand side of O.D.E.’s in 1 time step of R-K time advancing.

  FFT can be carried out efficiently on vector processors, or on the Earth simulator.

- Memory size is increased as \( O(N^3) \), where \( N \) is a number of grid points in one-direction.
Memory capacity required for a sequential version = $25N^3$

<table>
<thead>
<tr>
<th>$N^3$</th>
<th>$25N^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$512^3$</td>
<td>25 GB</td>
</tr>
<tr>
<td>$1024^3$</td>
<td>200 GB</td>
</tr>
<tr>
<td>$2048^3$</td>
<td>1.6 TB</td>
</tr>
<tr>
<td>$4096^3$</td>
<td>12.8 TB</td>
</tr>
<tr>
<td>$8192^3$</td>
<td>102 TB</td>
</tr>
</tbody>
</table>

Possible on ES!!

Double precision for Nonlinear term, but single for the linear term & R-K integration

7.2TB in Total

4096$^3$ DNS is possible on 512 nodes of ES
Implementation of a DNS code

- written in Fortran90.

- Eighteen 3D-FFTs are required for evaluations of the right hand side of O.D.E.’s in 1 time step of R-K time advancing

  \[ \text{FFT can be carried out efficiently on vector processors, or on the Earth simulator.} \]

- Memory size is increased as \( O(N^3) \), where \( N \) is a number of grid points in one-direction.

- 3D-FFT parallelized by domain decomposition needs all-to-all communications in transposing data distributed on the system

  \[ \text{High-speed data transfer is required.} \]
3D-FFT by domain decomposition

Fourier Space

\[ \hat{u}_{k_1, k_2, k_3} \]

FFT

Vector processing

Microtasking

MPI

Physical Space

\[ u_{j_1, j_2, j_3} \]

3D-FFT by domain decomposition

\[ V(\frac{N+1}{n_d}, N, N) \]

\[ V(\frac{N+1}{n_d}, N, N) \]

\[ V(\frac{N+1}{n_d}, N, N) \]

(FFT)

Microtasking

Vector processing

(FFT)

Microtasking

MPI

MPI

Microtasking

Microtasking

Microtasking
Points of Implementation (radix-4 FFT)

- Ratio of memory access to floating point operation is a critical issue on ES to keep performance high enough.
  - Peak performance of vector processor is 8 Gflops.
  - Bandwidth between a VP and main memory is 32 GB/s.
  - The ratio of the number of times memory is accessed to the number of floating point data operations is 0.5.

- Kernel code of radix-2 FFT shows the ratio as 1.

- Radix-4 or more FFT can be achieved higher performance, because the ratio is lower than 0.5.

Radix-4 FFT is taken in the implementation.
### Performance

Table 1: Performance in Tfllops of the computations with double [single] precision arithmetic as counted by the hardware monitor on the ES. The numbers in ( - ) denote the values for computational efficiency, $C_E$. The number $n_P$ of APs in each PN is a fixed 8.

<table>
<thead>
<tr>
<th>$N^3 \setminus n_d$</th>
<th>512</th>
<th>256</th>
<th>128</th>
<th>64</th>
</tr>
</thead>
<tbody>
<tr>
<td>2048^3</td>
<td>13.7(0.43)[15.3(0.48)]</td>
<td>6.9(0.43)[7.8(0.49)]</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>1024^3</td>
<td>11.3(0.35)[11.2(0.35)]</td>
<td>6.2(0.39)[7.2(0.45)]</td>
<td>3.3(0.41)[3.7(0.47)]</td>
<td>1.7(0.43)[1.9(0.48)]</td>
</tr>
<tr>
<td>512^3</td>
<td>–</td>
<td>4.1(0.26)[4.0(0.25)]</td>
<td>2.7(0.34)[3.0(0.38)]</td>
<td>1.5(0.38)[1.7(0.43)]</td>
</tr>
<tr>
<td>256^3</td>
<td>–</td>
<td>–</td>
<td>1.3(0.16)[1.2(0.15)]</td>
<td>1.0(0.26)[1.1(0.28)]</td>
</tr>
<tr>
<td>128^3</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.3(0.07)[0.3(0.07)]</td>
</tr>
</tbody>
</table>

Table 2: Performance in Tfllops as calculated for the same cases in Table 1 by using the analytical expressions for numbers of operations.

<table>
<thead>
<tr>
<th>$N^3 \setminus n_d$</th>
<th>512</th>
<th>256</th>
<th>128</th>
<th>64</th>
</tr>
</thead>
<tbody>
<tr>
<td>1024^3</td>
<td>12.2[12.1]</td>
<td>6.7[7.7]</td>
<td>3.5[4.0]</td>
<td>1.8[2.1]</td>
</tr>
<tr>
<td>512^3</td>
<td>–</td>
<td>4.4[4.3]</td>
<td>3.0[3.3]</td>
<td>1.7[1.9]</td>
</tr>
<tr>
<td>256^3</td>
<td>–</td>
<td>–</td>
<td>1.4[1.3]</td>
<td>1.1[1.2]</td>
</tr>
<tr>
<td>128^3</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.3[0.3]</td>
</tr>
</tbody>
</table>

From YIUIK(SC2002)
Calculation time of 1 time step

![Graph showing calculation time vs. number of PNs for different N values.]

- **Calculation Time**: 30.7 sec
- **Number of PNs**: About 3 days by 512 PNs for 1T (about 8400 steps)
Performance in Tflops

16.4Tflops
50% of the peak
(single precision & analytical FLOP number)
# Performance by VPP5000

<table>
<thead>
<tr>
<th>$N^3$</th>
<th>$256^3$</th>
<th>$512^3$</th>
<th>$1024^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td># of PE</td>
<td>16(8,4,2)</td>
<td>32(16,8,4)</td>
<td>32</td>
</tr>
<tr>
<td>Com. sped [1step]</td>
<td>4.45sec (10,23,48)</td>
<td>17sec (38,94,189)</td>
<td>160sec</td>
</tr>
<tr>
<td>Com. time</td>
<td>12h/20T</td>
<td>47h/20T</td>
<td>177h/5T</td>
</tr>
<tr>
<td>Required memory</td>
<td>2.7GB</td>
<td>22GB</td>
<td>176GB</td>
</tr>
<tr>
<td>I/O (time)</td>
<td>0.4GB (1)</td>
<td>3GB (7/5sec)</td>
<td>24GB (4/1min)</td>
</tr>
</tbody>
</table>
## Data Size & Transfer

3D-field, 1 snapshot, double(single) precision

<table>
<thead>
<tr>
<th>$N^3$</th>
<th>Data-Size</th>
<th>FTP with 10Mbps ~1MB/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>512$^3$</td>
<td>1 GB</td>
<td>16 min.</td>
</tr>
<tr>
<td>1024$^3$</td>
<td>8 GB</td>
<td>2.2 h</td>
</tr>
<tr>
<td>2048$^3$</td>
<td>64 GB</td>
<td>18 h</td>
</tr>
<tr>
<td>4096$^3$</td>
<td>(256GB)</td>
<td>3 days</td>
</tr>
</tbody>
</table>

$(u,v,w) +$ etc $\rightarrow$ 0.8TB
Conclusion I

• High Performance Computing (16.4TFlops)
  DNS of Turbulence in the $4096^3$ range

# of freedom = $2.5 \times 10^{11}$ with
Strong-Nonlinear, Non-Local Interaction
Dissipative Open system
II) Visualization
N=2048

from YIUIK(SC2002)
Image of Flow Field (Vorticity) by DNS with $N^3=2048^3$ from YIUIK(SC2002)
Close up view-1

from YIUIK(SC2002)
Close up view-2

from YIUIK(SC2002)
Close up view-3

from YIUIK(SC2002)
II) Some DNS Results
Energy spectrum & energy transfer

(at statistically steady state)

\[ \Pi(k) = \int_k^\infty T(k) \, dk \]

Some difference from DNS with lower resolution: -1

\[ k \eta \]

\[ C_K = 1.62 \pm 0.17 \quad \text{Experimental values (from Sreenivasan 1995)} \]

\[ C_K = 1.77 \quad \text{ALHDIA (Kraichnan 1966)} \quad C_K = 1.72 \quad \text{LRA (Kaneda 1986)} \]

\[ R_\lambda = 1450 \quad \text{S. G. Saddoughi and S. V. Veeravalli} \]

cf. I&K, Statistical Theories and Computational Approaches to Turbulence, Springer (2002), ed. YK & Gotoh, pp. 177

Not wide

Not flat
Some difference: -2

\[
\left( \frac{\partial}{\partial t} + 2\nu k^2 \right) E(k) = T(k)
\]

Energy Transfer

\[ T(k) \]

\[ -\Pi(k) \]

Not stationary

\[ \Pi \neq \varepsilon \]

cf. I&K, Statistical Theories and Computational Approaches to Turbulence, Springer(2002), ed. YK & Gotoh, pp.177
Analysis of the DNS data by ES

underway

• DNS’s up to $R_\lambda=1200$ suggest

  Normalized dissipation $\mathcal{E} \to \text{const}$, as $R \to \infty$

• Energy Spectrum
• Scaling & Statistics of 4th order velocity moments
  mean squares of $\nabla^2 p$, $\omega \cdot \omega$, $SS = \mathcal{E}/(2\nu)$

• High order structure functions,
  pdf, joint-pdf, intermittency
• Anisotropic scaling, effects of anisotropy,
• Inertial range structure,
• Dissipation range spectrum, 
• Direct & Qualitative Examination of Theories
Some difference from DNS with lower resolution: -2

\[ \Pi = \varepsilon \quad (\text{width, flat, stationarity}) \]

\[ \Pi(k) = \int_{k}^{\infty} T(k) \, dk \]

N=2048, \[ k_{\text{max}} \eta \sim 1 \quad R_{\lambda} \sim 732 \]

(from Phys Fluids 12(2003),L21-L24)
Normalized energy dissipation $\alpha \rightarrow ?$
as $\nu \rightarrow 0$, or $\text{Re} \rightarrow \infty$

$\alpha = \frac{eL}{u'^3}$

Approaches to a constant as $\text{Re} \rightarrow \infty$

(from Sreenivasan(1998), from I&K(2002)

(from Phys Fluids 12(2003), L21-L24)
FIG. 5: Compensated energy spectra from DNSs with (A) $512^3$, $1024^3$, and (B) $2048^3$, $4096^3$ grid points. Scales on the right and left are for (A) and (B), respectively.

(from Phys Fluids 12(2003), L21-L24)
**FIG. 6:** Local slope $\zeta(r)$ of $f_0(r)$ versus $r/\eta$. The inset is an enlargement of the range $40 < r/\eta < 500$. The straight line shows $\zeta(r) = 0.734$. $>2/3$

(from Phys Fluids 15(2003), L21-L24)
Normalized Spectra of $<(\nabla^2 p)^2>$, $\Omega$ and $D$

Spectra of $<(\nabla^2 p)^2>$

$\Omega$: Square of $\omega\omega$

$D$: Square of $SS=\varepsilon/(2\nu)$

Fig. 3. Normalized spectra (a) $\Omega(k)/(\nu^{-5} \langle \varepsilon \rangle^{5/4})$ and (b) $D(k)/(\nu^{-5} \langle \varepsilon \rangle^{5/4})$ versus $k\eta$ in Runs 256, 512, 1024 and 2048.

(from J.Phys.Soc Jpn (2003), 983-986)
Compensated Spectra of $\Omega$ and $D$

Fig. 5. $\Omega(k)$ (thick lines) and $D(k)$ (thin lines) spectra compensated by $R_\lambda^{-0.25}(k\eta)^{2/3}/(\nu^{-5}\langle \epsilon \rangle^7)^{1/4}$. (from J.Phys.Soc Jpn (2003), 983-986)
according to DNS

- Scaling of $\nabla^2 p$, $\omega \cdot \omega$ & SS = $\varepsilon/(2\nu) \rightarrow k^{\zeta}$
  - Anomalous scaling
  with $\zeta \sim 5/3$, $m<0$, $n<0$, $(m, n \neq 0 \sim -2/3 ?)$

A question: Why are they different?

**NOTE:** $\nabla^2 p = (1/2)\omega \cdot \omega - SS$,
$\nabla^2 p, \omega \cdot \omega$ & SS
$\rightarrow$ dimensionally the same; $\left(\frac{du}{dx}\right)\left(\frac{du}{dx}\right)$
(density ignored)
\[ A(k) = \langle f(k)f(-k) \rangle = ? \]

( \( f = -\nabla^2 p \), \( \omega \cdot \omega \), \( SS = \epsilon/(2\nu) \) )

- \( f(k) = -C_{abcd} \sum_{k=p+q} \Delta \Delta \Delta \Delta p_a q_b u_c(p)u_d(q) \)

for

(i) \( f = -\nabla^2 p \) \( \Rightarrow \) \( C_{abcd} = \delta_{ad} \delta_{bc} \)

(ii) \( f = \omega \cdot \omega \) \( \Rightarrow \) \( C_{abcd} = \varepsilon_{iac} \varepsilon_{ibd} = \delta_{ab} \delta_{cd} - \delta_{ad} \delta_{bc} \)

(iii) \( f = SS \) \( \Rightarrow \) \( C_{abcd} = (\delta_{ab} \delta_{cd} + \delta_{ad} \delta_{bc})/2 \)

\[ A = \langle f(k)f(-k) \rangle \]

\[ = \langle C_{abcd} \sum_{\Delta} p_a q_b u_c(p)u_d(q) f(k) \times C_{a'b'c'd'} \sum_{\Delta} p'_a q'_b u_{c'}(p')u_{d'}(q') \rangle \]

\[ = C_{abcd} C_{a'b'c'd'} \sum \sum p_a q_b p'_a q'_b < u_c(p)u_d(q) u_{c'}(p')u_{d'}(q') > \]
Conclusion III

• A new stage of DNS may
  “catch the tail” of universality/scaling?
  scaling range $r : L \gg r \gg \eta$ with $\Pi \sim \varepsilon$

  - $R_\lambda = 700 \sim 1200 > R_\lambda$ in Laboratory experiments

  $\rightarrow$ Direct & Quantitative Examination of Hypotheses/Theories such as K41, RSH, etc?
The End

Thank you for your attention!