In-situ analysis and visualization of massively parallel computations of transitional and turbulent flows

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Fluid Mechanics
Turbulent flows

Generation of turbulence behind a grid, T. Corke and H. Nagib in M. Van Dyke, 1982

Fluctuations over a wide range of non-linearly interacting scales

Understanding the physics of turbulence has very early involved direct numerical simulations
Direct Numerical Simulations (DNS)

⇒ Resolve all length and time scales

Navier-Stokes equations
Conservation of mass and momentum

\[ \partial_t \mathbf{U} + \mathbf{U} \cdot \nabla \mathbf{U} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{U} \]

\[ \nabla \cdot \mathbf{U} = 0 \]

(velocity \( \mathbf{U} \), pressure \( p \), density \( \rho \), viscosity \( \nu \))

+ initial and boundary conditions

⇒ Gives access to detailed physical quantities (beyond experiments)

⇒ Computationally intensive
How do flows become turbulent?

O. Reynolds’ pipe flow experiment (1883)

Observation of the laminar, transitional and turbulent flow regimes
Physical and computational challenge: 
**Numerical experiments of spatially evolving transitional and turbulent flows**
"High-Performance Computing is the use of super computers and parallel processing techniques for solving complex computational problems." (from Techopedia)

Constraints

- Numerical experiments require spectral accuracy
- Efficiency (follow flow development during long time)
Requires from 100 to 10000 cores

Large configuration in space and time

- 34560 × 192 × 768 modes (∼ 5. billions of modes)
- travel 1 length with nt=600000 time step.

Memory constraint

- \( N = N_x \times N_y \times N_z \), with \( N \) very large
  - large memory requirement (executable ∼ 2 To)
  - BlueGene/P 0.5 Go per core ⇒ ∼ **4000 cores needed**

Wall clock time constraint

- CPU time 150h ∼ 6 days on ∼ 16000 cores
  - with 100 cores (if possible), 160 times slower, 24000h ∼ 3 years
Big Data?

"Big data is a blanket term for any collection of data sets so large and complex that it becomes difficult to process using on-hand database management tools or traditional data processing applications. The challenges include capture, storage, search, sharing, transfer, analysis and visualization."
(from Wikipedia)

- An old (and recurrent) problem of fluid mechanics simulations
- But storage, network flow rate and connectivity grow more slowly than computation

⇒ Revisit traditional usage
Manage very large and highly partitioned files

<table>
<thead>
<tr>
<th>Large data</th>
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<tbody>
<tr>
<td>• 34560 × 192 × 768 modes</td>
</tr>
<tr>
<td>one velocity field occupies ( \sim 120 \text{ Go} )</td>
</tr>
<tr>
<td>statistics ( \sim 1 \text{ To} )</td>
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<table>
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<tr>
<th>Large amount of files, could rapidly exceeds inode or quota limit</th>
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<td>• statistics on ( \sim 2000 ) processes, ( \sim 16000 ) files</td>
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<tr>
<td>• need to write ( \sim 140 ) time step during travel length ( (L_x = 280) )</td>
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<td>(disk quota ( \sim 16 \text{ To} ))</td>
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• Data manipulation during simulation (checkpoint data)
• Data manipulation for analysis, post-treatment and visualization

⇒ **parallel strategy mandatory**
Spectral approximation

Spectral coefficients with $N_x \times N_y \times N_z$ modes

\[
U(x, y, z, t) = \sum_{m=-N_x/2}^{N_x/2} \sum_{p=-N_z/2}^{N_z/2} \left[ \sum_{n=0}^{N_y-1} \alpha_{OS,n}^m \hat{U}_{OS,n}^m + \sum_{n=0}^{N_y-1} \alpha_{SQ,n}^m \hat{U}_{SQ,n}^m \right]
\]

- Optimal representation of a solenoidal velocity field
- Elimination of the pressure

Spectral approximation

- Fourier-Chebyshev approximation with a Galerkin formulation
- Time integration with Runge-Kutta (3rd order)
Resolution of coupled systems for nonlinear advective terms

At each time step, $N_x \times N_z$ linear systems of dimension $N_y - 3$ are solved

\[ A_{OS}^{mp} \alpha_{OS}^{mp} = b_{OS}^{mp} \]
\[ A_{SQ}^{mp} \alpha_{SQ}^{mp} = b_{SQ}^{mp} \]

$A_{OS}^{mp}$ and $A_{SQ}^{mp}$ are sparse matrices (resp. 7D and 5D)

\[ b_{mp}^{mp} = b_{mp}^{mp}(\alpha_{SQ}^{mp}, \alpha_{OS}^{mp}) \]

contains non-linear terms
(consultation products coupling every $\alpha_{n}^{mp}$)

⇒ $b$ is calculated in physical space (pseudospectral method)
⇒ must perform FFTs in each direction

At each time step, 27 FFT (direct or inverse) are performed (∼16 millions of FFT)
2D domain decomposition

- Chebyshev between walls (y direction, $N_y + 1$ modes)
- 2D FFT in periodical directions (x direction and z direction)
- Transpose from $y$–pencil to $x$–pencil, $x$–pencil to $z$–pencil and back

Increase the number of MPI processes and reduce wall clock time

- 1D decomposition: $\text{MPI} \leq N_y$
  $34560 \times 192 \times 768 \rightarrow \text{max. of MPI processes: } nproc=192$
- 2D decomposition: $\text{MPI} \leq N_y \times N_z$
  $34560 \times 192 \times 768 \rightarrow \text{max. of MPI processes: } nproc=147456$
- Perform data communications and remapping
- Choose data rearrangement to limit the increase in communications
Constraints related to modern many-cores platforms

Tendancy towards many-cores platforms

- Limited number of nodes
- Increase of cores per node (BlueGene/P = 4 - SuperMUC = 16)

Increase MPI processes

- allow larger number of modes within the same wall clock time
- limit the memory available per processus
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Hybrid OpenMP/MPI

**Suitable for recent many-core platforms**

- Reduces the number of MPI processes
  - Reduces the number of communications
  - Increases the available memory size per node

**Modification for many threads**

- Time of thread creation exceeds inner loop time execution
- Implementation of explicit creation of threads
- Recover full MPI performance and allow further improvement.
More than domain decomposition ...

Tasks parallelization: overlap communication by computation

- reduces by 20% time per time step

Placement of processes

- specific on each platform, optimize interconnection communications
- avoid threads to migrate from one core to another
  example: TORUS versus MESH in BlueGene/P platform - 50% faster
Speedup, efficiency and wall-clock time per time step

- 88% of efficiency on 16384 cores
- 0.2 s/dt sur SuperMUC for $10^9$ modes on 16384 cores
Data manipulation during simulation

I/O and storage

- Fast parallel I/O using standard XML/VTK or HDF5 format
  beware not to add useless complexity for regular structured data
- Unix I/O faster than MPI I/O (2x)
  in our experience on large HPC platforms
- I/O files embedded in a tar file (pvd + parallel vtr) or in a separate directory
  to avoid exceeding inodes number and fasten transfer
- perform FPZIP compression if needed (lossless or lossy (48bits))
  ⇒ Optimize data transfert between platform
  or perform co-analysis of the flow without writting raw data
Data manipulation after simulation

Data processing

- Part of the analysis is performed during simulation
- Part of it is explored afterwards

3D visualization

- Cannot be performed directly on HPC platforms

Requirements and constraints

- Entails spatial derivation, eigenvalues evaluation ...
- Preserve accuracy of the simulation
- Should be interactive and when ready on batch mode
Client/server workflow

HPC platform (Tier-0, Tier-1)

parallel transfer (GridFTP, ...)

data server

HPC cluster (Tier-2)

NFS

ssh tunneling

NFS

NX (x2go)/vnc

user

graphic stations (Tier-2)
Analysis and visualization of stored data

A posteriori on raw data (in parallel)

- Python script with mpi4py
- parallel client server with 2D/3D (matplotlib, mayavi)
- interface with C++ lib using swig
- manipulate tar data file
- analyze with simpler parallel partitioning (1D)
- preserve the same accuracy in the compute and analyze steps

- Still requires disk I/O, data transfert and storage
- Data storage and post-treatment identified as a major challenge

*S. Requena, Big Data and HPC, 2013*
In situ (real computational time) analysis and visualization

Remote co-processing during simulation without I/O of raw data

**Analysis**
Compute density energy spectra, statistics, etc. at physical relevant stride

**3D visualization**

**Open-source software**
- VisIt
- ParaView

**Requirements**
- Preserve spectral accuracy
- Computation of quantities from simulations variables
- Fast enough
- Act on simulation parameters (like in experiment)

**Limitations**
- run with the same granularity as the simulation
- affect speed of computation
Present in situ workflow

NS solver
C++ library
highly parallel compute
and I/O kernel

Analysis
python
parallel lib
numpy, mpi4py

Tools:
git
CMake/CTest
MPI/OpenMP
FFTW, BLAS
SWIG

compute nodes
control nodes
tar file

Anysynchronous analysis

<table>
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<tr>
<th>NS solver</th>
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<td>analyse</td>
<td>analyse</td>
<td>...</td>
<td>analyse</td>
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Example: visualization of sinuous/varicose instabilities

Control of the numerical experiment:
modification of the amplitude of the perturbation at the channel entry while the simulation is running
Benefits of the new implementation

- Simplify the analysis
- Get faster developments and tests
- Make overlap I/O and computation, asynchronous execution and communications
- Allow in-situ visualization
- but need a more complex environment!
  - coupling between C++/python/external tools (VisIt)
  - asynchronous communications
  - depend on a large number of external libraries (compatibility)
  - make the porting and tuning on HPC platforms more complex
    limitation of the module system
What was achieved for HPC simulations

A suitable development and software environment

- code C++
- BLAS, GSL
- MPI/OpenMP - optimized libraries (e.g. FFTW, MKL)
- cmake, git
  - swig interface Python and a C++ library derived from the code
  - python, mpi4py, numpy, matplotlib, mayavi, visit ...

Development of a parallel strategy for the code

- revisit parallel strategy of the code
- revisit strategy of data transfer and storage
- revisit strategy for the analysis and visualization