Fluid Mechanics and HPC
Successes, Challenges, and Future Prospects

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DNS of turbulence during the intake stroke of the TCC-3 engine model. G. Giannakopoulos
Outline

- Objectives
  - Computational landscape

- Successes
  - Predictive?

- Challenges

- Future Prospects

Thanks Bob!! 😊
This Talk: A View through a Single Lens

Nek5000

- Spectral Element Discretizations
- High-order Timesteppers
- Multilevel Solvers
- Scalable Implementations

NekCEM

- Vascular flow
- Magneto-Rotational Instability
- Reactor Thermal Hydraulics
- Combustion in IC engines etc. …
**Incompressible Navier-Stokes Equations**

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}
\]

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

- **Key algorithmic / architectural issues:**
  - Unsteady evolution implies many timesteps, significant reuse of preconditioners, data partitioning, etc.
  - \(\text{div } \mathbf{u} = 0\) implies *long-range global coupling at each timestep*
    \[\rightarrow \text{iterative solvers}\]
    \[\rightarrow \text{communication intensive}\]
  - Small dissipation \(\rightarrow\) large number of scales \(\rightarrow\) large number of gridpoints for high Reynolds number \(Re\)

- Complex geometries and BCs keep everything interesting.
**Industrial Example**

- 12 hour turnaround for result on the left:
  - 6 hours to mesh, 6 hours to run on 16K cores
- 3 Days for result on the right (mostly meshing...)
DNS of Flow around a NACA4412 Wing Profile

Re_c = 400,000 with 5° angle of attack.
3.2 billion gridpoints

Enhanced cooling for ANL’s Advanced Photon Source

w/ J. Collins, ANL-APS

- Front-end and beam-line high thermal-load devices.
  - Wire-coil inserts increase heat transfer up to 4X over straight passages.
  - CFD lends insight into enhancement mechanisms.
Results, for similar geometry, full conjugate heat transfer:

- Excellent prediction of heat transfer coefficient.
- Analysis, however, is perplexing because of a large region of negative eddy diffusivity.
- We’ve recently realized that this is not uncommon in oscillatory systems.
- The insight has led to potential design improvements, currently being simulated.
Sublaminar Drag in Curved Pipe Flow
— Noorani & Schlatter ’12

DNS results are being used to calibrate new RANS models in commercial engineering codes.

10% drag reduction!

Tangential Velocity (symmetry plane) shows clear wave pattern

(last 48 hours)
Transition in Arterio-Venous Grafts

- Port for dialysis patients: sustain high flow rates → efficient dialysis

- PTFE plastic tubing surgically attached from artery to vein
  - short-circuit of high- to low-pressure vessels yields high velocities—weak turbulence

- Graft failure results in 50% of cases after 3-6 months due excessive stimulation and growth of smooth muscle cells (intimal hyperplasia) downstream of attachment to vein.
Where is the Turbulence Coming From?

- Flow reversal (upstream), into DVS
  - Three simulations with steady inlet conditions at $Re_G = 1200$
  - 100, 85, and 70% flow through PVS
  - 70% case shows strong turbulence, despite the fact that $Re_{PVS} = 950$
  - Results confirmed by LDA measurements in the same geometry.
Mean Flow for Re 1200, 70:30 Flow Split

Comparison of spectral element and measured velocity distributions in an arteriovenous graft, $Re_G = 1200$

Coherent structures in arteriovenous graft @ $Re_G = 1200$

(Computations by S.W. Lee, UIC. Experiments by D. Smith, UIC)
Influence of Reynolds Number and Flow Division on $u_{rms}$
Reactor Examples

- Thermal striping in a T-Junction
  - Important because thermal stresses lead to component failure
  - Subject of OECD/NEA-sponsored blind-benchmark

- ANL Max Experiment
  - Thermal striping mock-up of outlet plenum
    - co-flowing jets at different temperatures

- Rod bundle flows
  - Transition / mixing / RANS validation
Thermal striping leads to thermal fatigue in structural components

Centerplane, side, and top views of temperature distribution
Nek5000 Submission to T-Junction Benchmark

- E=62000 spectral elements of order N=7 (n=21 million)
- \( \text{Re}_D = 40,000 \) for inlet pipes
- Subgrid dissipation modeled with low-pass spectral filter
- \( L_x \sim 25 D \) (cost is quadratic in \( L_x \))
- 24 hours on 16384 processors of BG/P (850 MHz) \( \sim 33x \) slower than uRANS

Recycling turbulent inflows

Test Section, \( L_x \)
Results Presented by NEA/OECD Benchmark Organizers

- Experiment with hot/cold inlets at Re ~ 10^5
- Velocity and temperature inlet data provided by Vattenfall.
- 29 entries, resolution n=1 to 70 M gridpoints
- SEM ranked 1st in thermocouple prediction
Argonne is constructing a highly instrumented experiment (MAX) to provide detailed velocity and temperature data for code validation.

- 1 x 1 x 1.7 m$^3$
- High speed thermal imaging camera
- PIV

Figure 1. Apparatus for gas mixing experiments: Nd:YLF laser (left), infrared camera (top), PIV camera (right), and hexagonal flow channels (below).
**MAX Experiment: LES / RANS Comparisons**

- **Steady RANS about 100,000 X faster than LES**

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Merzari et al., On the numerical simulation of thermal striping in the upper plenum of a fast reactor, ICAPP (2010)
**Why High-Fidelity?**

**Major Difference in Jet Behavior for Minor Design Change!**

**Simulation Results:**
- Small perturbation yields $O(1)$ change in jet behavior
- Unstable jet, with low-frequency (20 – 30 s) oscillations
- Visualization shows change due to jet / cross-flow interaction
- MAX2 results **not** predicted by steady RANS (URANS ok)

Lomperski et al., *Jet stability and wall impingement flow field in a thermal striping experiment*, IJHMT 115 (2017)
Time Series Analysis of MAX Data

- MAX1 – **STABLE:** canisters extending into the domain
- MAX2 – **UNSTABLE:** canisters flush with plenum floor
  - Order-unity oscillations in jet position
  - Implications for thermal striping (thermal-mechanical fatigue)

Energy Spectrum

- ~20 seconds
- .06 Hz
- $k^{-5/3}$
MATIS Benchmark Problem

A. Obabko

- 220 million points
- 400,000 elements
- 5 million CPU hrs

- Ranked first in prediction of turbulence rms
A Sobering Fact: We Are Not Running Faster

**Panda Thermal Stratification Benchmark**
(Obabko, Tomboulides, Aithal, Merzari, F. 2014)

- Low density jet entering stratified background
- Very long time integrations
  - 1 month of wall clock time
  - 2 minutes of physics
  - Desire 2 hours \(\rightarrow\) **5 years wall-clock time on 8K cores.**
- Nek5000
  - \(n \sim EN^3 = 62\text{ million gridpoints}\)
  - \(P = 16384\text{ MPI ranks}\)
  - \(n / P \sim 3000\)
- For straight hydro, cannot further reduce \(n/P\)
A Computational Quandary

- We are not running faster

  - Clock speeds are fixed at ~ 1 – 4 GHz for past 10 years
  - Power concerns favor reduced clock speeds and more parallelism.
  - Communication costs limit granularity to be relatively coarse.

- What can we do?

<table>
<thead>
<tr>
<th>Time Savings</th>
<th>Power Savings</th>
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<tbody>
<tr>
<td>High-Order</td>
<td>10 x</td>
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<tr>
<td>Scalable solvers</td>
<td>10 x</td>
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<tr>
<td>Lower communication costs</td>
<td>10 x</td>
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<tr>
<td>Parallel in time? (ensemble average?)</td>
<td>10 x</td>
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<tr>
<td>Lower $n_{1/2}$ on nodes</td>
<td>? x</td>
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Influence of Scaling on Discretization

Large problem sizes enabled by peta- and exascale computers allow propagation of small features (size $\lambda$) over distances $L >> l$. If speed $\sim 1$, then $t_{\text{final}} \sim L/\lambda$.

- Dispersion errors accumulate linearly with time:

$$\sim |\text{correct speed} - \text{numerical speed}| * t \quad \text{(for each wavenumber)}$$

$$\rightarrow \text{error}_{t_{\text{final}}} \sim (L/\lambda) * |\text{numerical dispersion error}|$$

- For fixed final error $\varepsilon_f$, require: numerical dispersion error $\sim (\lambda/L)\varepsilon_f, << 1$.

High-order methods can efficiently deliver small dispersion errors.

(Kreiss & Oliger 72, Gottlieb et al. 2007)
High-Order Spatial Discretizations

Example: Spectral element method (Patera 84, Maday & Patera 89)

- Variational method, similar to FEM, using GL quadrature.
- Domain partitioned into $E$ high-order hexahedral elements
- Trial and test functions represented as $N$th-order tensor-product polynomials within each element. ($N \sim 4 -- 15$, typ.)

- $n \sim EN^3$ gridpoints in 3D
- Fast operator evaluation: $O(n)$ storage, $O(nN)$ work
- Converges \textit{exponentially fast} with $N$ for smooth solutions.

2D basis function, N=10
Spectral Element Convergence: Exponential with $N$

- 4 orders-of-magnitude error reduction when doubling the resolution in each direction

- For a given error,
  - Reduced number of gridpoints
  - Reduced memory footprint.
  - Reduced data movement.

Exact Navier-Stokes Solution (Kovazsnay ‘48)

$$v_x = 1 - e^{\lambda x} \cos 2\pi y$$

$$v_y = \frac{\lambda}{2\pi} e^{\lambda x} \sin 2\pi y$$

$$\lambda := \frac{Re}{2} - \sqrt{\frac{Re^2}{4} + 4\pi^2}$$
Excellent transport properties, even for non-smooth solutions

Convection of non-smooth data on a 32x32 grid. (cf. Gottlieb & Orszag 77)

(K₁ x K₁ spectral elements of order N)
**Stabilization via Spectral Filter**

Boyd ’98, F. & Mullen ‘01

- Expand in modal basis:
  \[ u(x) = \sum_{k=0}^{N} \hat{u}_k \phi_k(r) \]

- Set filtered function to:
  \[ \tilde{u}(x) = \tilde{F}(u) = \sum_{k=0}^{N} \sigma_k \hat{u}_k \phi_k(r) \]

- Spectral convergence and continuity preserved. (Coefficients decay exponentially fast.)

- In higher space dimensions:
  \[ F = \tilde{F} \otimes \tilde{F} \otimes \tilde{F} \]
Figure 6: Eigenmodes for free-surface film flow: (left, top) contours of vertical velocity $v$ for unfiltered and (left, bottom) filtered solution at time $t = 179.6$; (right) error in growth rate vs. $t$.

Filtering permits $Re_{d99} > 700$ for transitional boundary layer calculations.

Figure 1: Principal vortex structures identified by $\lambda_2 = -1$ isosurfaces at $Re = 700$: standing horseshoe vortex (a), interlaced tails (b), hairpin head (c), and bridge (d). Colors indicate pressure. ($K=1021$, $N=15$).
Hairpin Vortices in an Intake Port

- $Re_D = 45,000$
- Note the highly-resolved filamental horseshoe vortices around the base of the valve stem that ultimately break down into a hairpin vortex chain.
- Although turbulent, it’s definitely not *random*!
The Success of Filtering Led us to Understand a Major Source of Instability –

**Aliasing in Advection:** \( u_t + c \cdot \nabla u = 0 \)

- Velocity fields model first-order terms in expansion of straining and rotating flows.
- Rotational case is skew-symmetric.
- Aliasing is not a nonlinear phenomena. (*This problem is linear.*)
- Filtering attacks the leading-order unstable mode.

\[
\begin{align*}
&\text{c = (-x,y)} \\
&\text{c = (-y,x)}
\end{align*}
\]

Aliased / Dealiiased Eigenvalues

*Malm et al., JSC 2013*
Cost Driver: Scalable Multilevel Solvers:
Cost Driver: Scalable Multilevel Solvers:

\[ \mathbf{z} = \mathbf{M}\mathbf{r} = \sum_{e=1}^{E} \mathbf{R}_e^T \mathbf{A}_e^{-1} \mathbf{R}_e \mathbf{r} + \mathbf{R}_0^T \mathbf{A}_0^{-1} \mathbf{R}_0 \mathbf{r} \]

(Dryja & Widlund 87, Pahl 93, Lottes & F 01)

Local Overlapping Smoother: FEM-based Poisson problems with homogeneous Dirichlet boundary conditions, \( \mathbf{A}_e \).

Use fast diagonalization.

Coarse Grid Solve: Poisson problem using linear finite elements on entire spectral element mesh, \( \mathbf{A}_0 \) (GLOBAL).
Putting At All Together: Subassembly with 217 Wire-Wrapped Pins

- 3 million 7th-order spectral elements (n=1.01 billion)
- 16384–131072 processors of IBM BG/P
- 15 iterations per timestep; 1 sec/step @ P=131072
- Coarse grid solve < 10% run time at P=131072
Scaling to Beyond 1 Million Processes

217 Pin Problem, N=9, E=3e6:

- 2 billion points
- BGQ – 524288 cores
  - 1 or 2 ranks per core
- A mixture of CG / multigrid
- 60% parallel efficiency at 1 million processes
- 2000 points/process
Some Exascale Questions

- Will this scaling continue as we move to exascale?
- Is this the best we can do?
- What, exactly, is better, or even good?
  - Good node performance
  - Strong scaling to large processor counts.

Strong scaling is ultimately limited by costs that do not go to zero as $n/P \to 0$:

$$t \sim c_1 \frac{n}{P} + c_2 + c_3 \log P$$

- $c_2 \sim$ communication overhead
  - $\sim$ other overhead (memory latency on GPU)
  - $\sim$ Amdahl
- $c_3 \sim$ can be mitigated by hardware on the NIC

Analyze through modeling computational complexity.
Complexity Models for Iterative Solvers

- Point Jacobi iteration (7-point stencil, 3D):
  - Work: \( T_{aJ} \sim 14 \frac{n}{P} t_a \)
  - Communication: \( T_{cJ} \sim (6 + (\frac{n}{P})^{2/3} (\frac{1}{m_2})) \alpha t_a \)

- Conjugate gradient iteration (7-point stencil): (alt: Chebyshev iteration)
  - Work: \( T_{aCG} \sim 27 \frac{n}{P} t_a \)
  - Communication: \( T_{cCG} \sim T_{cJ} + 4 \log_2 P \alpha t_a \)

- Geometric Multigrid:
  - Work: \( T_{aMG} \sim 50 \frac{n}{P} t_a \)
  - Communication: \( T_{cMG} \sim (8 \log_2 \frac{n}{P} + 30m_2 (\frac{n}{P})^{2/3} + 8 \log_2 P) \alpha t_a \)
Scaling Estimates: Jacobi

Q: How large must n/P be for $T_a \sim T_c$?

$$\frac{T_c}{T_a} = \frac{6 \left(1 + \frac{1}{m_2} (n/P)^{2/3}\right) \alpha}{14 n/P} \leq 1$$

$\alpha = 2300$

$\beta = 12.6$

$m_2 = 185$

$(n/P) \approx 2000$

- Similar analysis leads to
  - $n/P \approx 1200$ for CG
  - $n/P \approx 12,000$ for multigrid
  - Consistent with observed scaling behavior
We are interested in high performance for relatively small local problem sizes.

In HPC, we need to keep an eye on not only (application-specific) peak sustained node performance, $S_1$.

We also need to be concerned with how large the local problem size must be to reach the saturated performance limit.

At the strong-scale limit, time to solution scales like:

$$T_P \sim O\left( \frac{n_{1/2}}{S_1} \right)$$

Increasing $S_1$ reduces time to solution only if $n_{1/2}$ does not rise commensurately.

Obviously, this argument doesn’t address power/cost concerns.
Recent Production Runs at 1 Million Ranks

A. Obabko

- Conjugate heat transfer
  - Seven pitches
  - E=15 million elements
  - N=5
  - n=1.5 billion
  - time in coarse solve: 19 & 26%

- Runs on 16 and 32 racks BGQ
  - P=524288 and 1048576 ranks
  - n/P = 2861 and 1430
  - $\eta_P = .72$ and .56
  - Very close to earlier performance model
Summary & Observations

- We have come a long way in predictive turbulence simulations.

- Long-time integrations continue to put pressure on the need for strong scaling:
  - more processors for fixed problem size
  - \( n/P \to 0 \)

- New complex nodes are driving \( n/P \gg 1 \).
  - \( n_{1/2} \) limits
  - potential adverse impact on running fast

- Ensemble averaging and reduced-order models are possible mitigation strategies.
Thank you Bob for making this an energetic and successful enterprise!