Extreme-scale computing and studies of intermittency, mixing of passive scalars and stratified flows in turbulence

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Ph.D. Thesis Defense

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Outline

- Introduction
- GPU acceleration of pseudo-spectral turbulence simulations
- Understanding intermittency through extreme-scale computation
- Extreme dissipation and its multifractal nature at high Reynolds numbers
- High resolution studies of intermittency in scalar dissipation rates
- Active scalar turbulence
- Conclusions and Future directions

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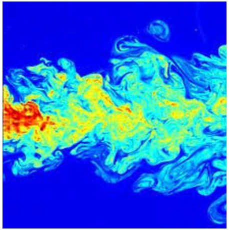
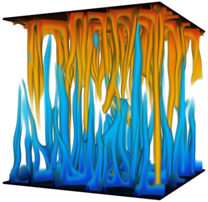
Turbulence

- A physical problem of great complexity, and a critical factor in many disciplines
- Disorderly fluctuations over a wide range of scales in 3D space and time





- Pseudo-spectral Direct Numerical Simulations: a powerful investigative tool
- Extreme fluctuations in velocity gradients: stringent resolution requirements
- Agent of efficient mixing of substances and properties

Extreme-scale computing for turbulence

Communication intensive code (e.g. 3D FFT) on heterogeneous machines?

- accelerators provide most of computing power, but need to move data
- communication still an issue (perhaps even more so): some new challenges

Achieve extreme problem sizes without being limited by GPU memory?

- process data in batches on GPU with entire data residing in CPU memory
- potential for asynchronous operations; optimize the data copies

Code developments on Summit (IBM+NVIDIA) used CUDA Fortran

- Future exascale machine, Frontier: AMD hardware, CUDA Fortran not supported
- portability: using OpenMP to program GPUs, up to Version 5.0

Need new algorithms for large scale runs on heterogeneous machines

Understanding intermittency using high resolution simulations

High resolution simulations are often short due to finite resources

- Particularly for flows at high Reynolds numbers (R_λ)
- Simulations of short duration useful in studying small-scales which evolve quickly
- Statistical sampling and independence is a concern

Average data from multiple resolution independent simulations (MRIS)?

- Each short simulation with grid refinement starts from lower resolution snapshot
- Initial snapshots used are spaced out in time for better independence

Study effects of intermittency using MRIS approach up to $R_\lambda \sim 1300$

- Validation of MRIS for use in studies of small-scale
- Statistics of dissipation rate and enstrophy averaged over 3D sub-domains

New protocol for large simulations to study fine-scale intermittency

Energy dissipation rate and its multifractal nature

Describe highly intermittent quantity like energy dissipation?

- Fluctuations as large as 1000 times the mean expected, especially at high R_λ
- Unlike near-Gaussian processes, low-order moments cannot describe it completely

Turbulence under a multifractal framework (Sreenivasan 1991)

- Fractals: objects with self-similar properties over wide range of scales
- Complex process like turbulence: multifractal spectrum, set of “fractal dimensions”

High resolution data from MRIS work: compute multifractal spectrum

- High-order moments of 3D local averages energy dissipation: extrapolation of PDF
- For $R_\lambda \sim 390$ to 1300: effect of R_λ on multifractal spectrum

Fine-scale intermittency of energy dissipation: multifractal approach

High resolution studies of passive scalar intermittency

Turbulent flows: an agent of efficient mixing of substances or properties

- Low concentration, does not affect the flow: passive scalars ($Sc = \nu/D$)
- Focus on $Sc \sim \mathcal{O}(1)$, typical of gas-phase mixing

Large fluctuations of energy and scalar dissipation rates

- Can lead to inefficient combustion, chemical processes, etc
- How do energy and scalar dissipation rates relate to each other?

High-resolution DNS help capture extreme events accurately

- Average over multiple short independent simulations (Yeung *et al.* 2020)
- Study intermittency: moments of 3D local averages and conditional moments

Understand intermittent nature of small-scale in passive scalar field

Active scalar turbulence and double diffusive phenomena

Density stratification in the presence of two active scalars

- Strength of stratification: Froude number (buoyancy to turbulence time scales)
- Density variations give rise to buoyancy forces: Boussinesq approximation

Buoyancy effects can be stabilizing or destabilizing

- Two scalars with opposing effects: differential diffusion pivotal role
- Strong unstable stratification: stricter spatial and temporal resolution constraints

Evolution of anisotropy and double-diffusive convection

- Flow energetics and nature of Reynolds-stress budget

Understand anisotropy development and differential diffusion effects

Objectives

Develop algorithm capable of extremely large scale DNS using GPUs

- Optimizing network communication and GPU-CPU data movements
- Track Lagrangian fluid particles using GPUs
- Address portability issues arising from heavy use of CUDA Fortran

Study intermittency & multifractal nature of energy dissipation

- Address sampling limitations due to short simulations at large scale
- Investigate extreme fluctuations of (scalar) dissipation and enstrophy, statistics of local averages, resolution effects in capturing extreme events
- Compute multifractal spectrum of energy dissipation rate

Study turbulence with density stratification due to two active scalars

- Two active scalars of opposing effects: anisotropy and differential diffusion effects

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Navier-Stokes equations and Fourier pseudo-spectral methods

- Numerical solution of PDE governing velocity field $\mathbf{u}(\mathbf{x}, t)$

$$\partial \mathbf{u}/\partial t + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla(p/\rho) + \nu \nabla^2 \mathbf{u} + \mathbf{f}$$

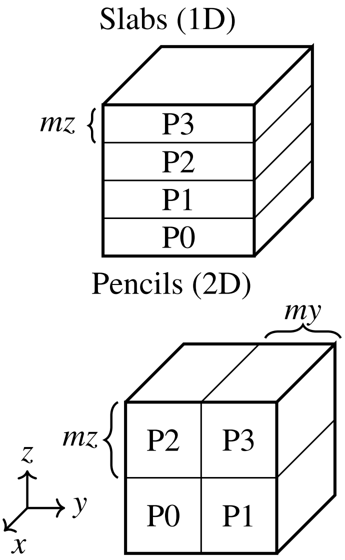
- Fourier decomposition: $\mathbf{u}(x, t) = \sum_{\mathbf{k}} \hat{\mathbf{u}}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x})$. In equation for Fourier coefficients nonlinear terms lead to convolution integrals, requiring $\sim N^6$ operations
- Pseudo-spectral: form products first by multiplication in physical space, before transforming to wavenumber space. Fast Fourier Transform (FFT) $\propto N^3 \ln_2 N$ — but communication is required to make complete lines of data available.
- Aliasing errors in nonlinear terms: use truncation and phase-shifts (Rogallo 1981)
- Cost of simulation per step tied to a number of forward and backward transforms.

Efficient distributed 3D FFT on GPUs forms a key component

Domain Decomposition: 1D or 2D?

How best to distribute memory among P MPI tasks?

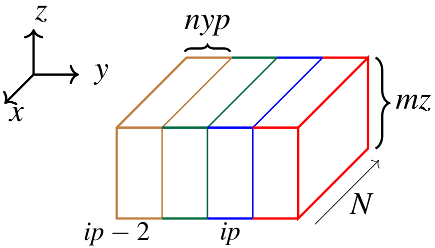
- 1D: Each MPI rank holds a slab
  — one global transpose among all processes ($x-y$ to $x-z$)
- 2D: Each rank holds a pencil
  — two transposes, within row and column communicators
- Pencils used for most large simulations (e.g. we ran 8192^3 using 262,144 MPI tasks on Blue Waters at NCSA)
- Fatter nodes and more GPUs per node: return to slabs?
  — GPU parallelism instead of distributed memory (MPI)
  — fewer nodes (and MPI tasks) in communication
  — associated pack and unpack operations are simplified



New batched asynchronous algorithm

Run large problem sizes efficiently without being limited by GPU memory

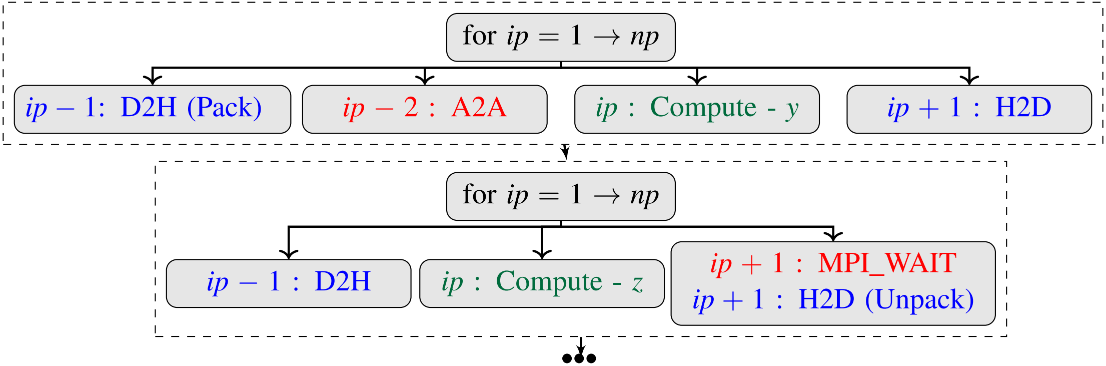
- Divide slab into np pencils ($N \times nyp \times mz$) and process each pencil separately ($nyp = N/np$)
- Overlap operations on different pencils to hide some data transfer and compute costs



Asynchronous execution using CUDA streams and events

- One compute stream and one data transfer stream — compute and data transfers can occur simultaneously
- CUDA events are used to enforce synchronization between streams

Batched asynchronism: Illustrated via operations in y and z



- Operations on same row executed asynchronously but launched from left to right
- Pack and unpack: strided data copy to avoid reordering data before transpose
- Non-blocking all-to-all allows overlap. Call MPI_WAIT before compute

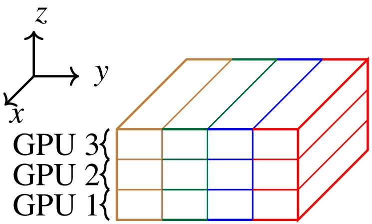
How many tasks per node?

Based on Summit node architecture

- 6 tasks per node: 1 task per GPU
- 2 tasks per node: 3 GPUs per task
  - — OpenMP threads to launch operations to GPUs
  - — 3 times fewer MPI tasks, 3 times larger message size

Number of pencils per all-to-all

- Does it affect the performance?
- 1 pencil at a time
  - — overlap MPI with data movement and compute
- Entire slab (*np* pencils) at a time
  - — no MPI overlap with data movement and compute
  - — *np* times larger message size and fewer MPI calls



Each pencil further divided vertically among multiple GPUs

MPI configurations test and performance

Test standalone blocking MPI all-to-all code to understand performance of configurations

Nodes	6 tasks/node 1 pencil/A2A		2 tasks/node 1 pencil/A2A		2 tasks/node 1 slab/A2A	
	P2P (MB)	BW (GB/s)	P2P (MB)	BW (GB/s)	P2P (MB)	BW (GB/s)
16	12	36.5	108	43.1	324	43.6
128	1.5	24.0	13.5	39.0	40.5	39.0
1024	0.19	11.1	1.69	23.5	5.06	25.0
3072	0.053	13.2	0.47	12.4	1.90	17.6

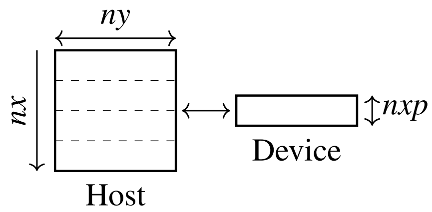
P2P reduces
BW reduces

Peer-to-Peer (P2P) size increases
Higher effective bandwidth (BW)

Trade-off: 1 pencil/A2A with overlap or 1 slab/A2A without overlap

Strided copy optimization

- Frequent strided copies required
  — computing on small pieces of data
  — pack/unpack data for MPI all-to-all
- Transform in y direction on $x - y$ slabs, with memory contiguous in x
- Many cudaMemCpyAsync: high overhead
- Pack data and transfer: addl. buffer on GPU



Contiguous Memory in x

Is there a faster way?

- zero-copy kernel (ZC): GPU initiates many small transfers to/from host page-locked (pinned) memory [Appelhans GTC 2018]
  — CUDA threads copy data CPU $\Longleftrightarrow$ GPU by directly accessing host resident memory
- cudaMemCpy2D (Cpy2D): API, accepts arguments to perform simple strided copies

Batched asynchronous code performance

- Performance data collected on Summit
  — 2nd order Runge Kutta, 3 inverse and 5 forward transforms, 2 substages per timestep

Nodes	Problem Size	Time(s)			
		Sync CPU (Pencils)	Async GPU		
			6 tasks/node	2 tasks/node	
				1 pencil/A2A	1 slab/A2A
16	3072^3	34.38	8.09	6.70	7.50
128	6144^3	40.18	12.17	8.66	8.07
1024	12288^3	47.57	13.63	12.62	10.14
3072	18432^3	41.96	25.44	22.30	14.24

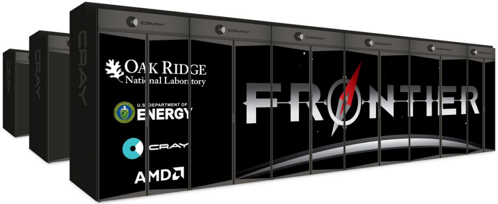
- 2 tasks/node performs better than 6 task/node for all problem sizes tested
- 128 nodes and above: 1 slab/A2A better than 1 pencil/A2A
  — suggests better overall performance without MPI overlapping GPU operations
- $18{,}432^3$: $\sim$ 3X speedup to pencils CPU version; communication bound code

Particle tracking algorithm using GPUs

- Lagrangian framework: follow particles moving with the (instantaneous) flow
- Compute flow field on fixed 3D grid, interpolating key quantities at particle position
- Cubic spline interpolation: solve linear tridiagonal systems successively in each coordinate direction — from N^3 grid to $(N+3)^3$ spline coefficients ($e_{ijk}(\mathbf{x})$)
- Workflow to compute 3-D spline coefficients similar to 3-D FFTs
  — 1-D spline coefficient in each direction, with all-to-all: batched asynchronism
  — GPUs to compute 1-D spline coefficients, strided copies for batches
- Interpolated velocities using spline coefficients (e_{ijk}) and basis functions (b_i, c_j, d_k)
  $$u^+ = \sum_{k=1}^{4} \sum_{j=1}^{4} \sum_{i=1}^{4} b_i(x^+) c_j(y^+) d_k(z^+) e_{ijk}(\mathbf{x})$$
- Local decomposition (Buaria *et al.* 2017): process tracks particles in its sub-domain
  — One-sided MPI to form Ghost layers; particles at sub-domain boundaries

Use GPUs to target trillions of grid points and billions of particles

Porting to future exascale architectures



- AMD CPU w/ 4 AMD GPUs per node
- Program GPUs: HIP, OpenMP

- 2 Intel CPUs w/ 6 Intel GPUs per node
- Program GPUs: oneAPI, OpenMP

Support for CUDA Fortran is not likely. Need efficient portable implementation.

OpenMP is widely accepted standard and a clear favorite for Fortran

- Ensure proper interoperability b/w OpenMP TASKs and GPU numerical libraries?

DETACH to enforce synchronization

```
TARGET DATA MAP(tofrom: a)

TASK DEPEND(out:var)  DETACH(event)

TARGET DATA USE_DEVICE_PTR(a)   Ⓐ
FFTExecute (a, forward, stream)
FFTExecute (a, inverse , stream)
END TARGET DATA

 hipStreamAddCallback (stream, ptr_callback, C_LOC(event), 0)
END TASK

! Copy or compute on other data   Ⓒ

TARGET TEAMS DISTRIBUTE DEPEND(IN:var) NOWAIT
a (:, :, :) = a (:, :, :) /nx                          Ⓑ
END TARGET TEAMS DISTRIBUTE

END TARGET DATA
```

```
subroutine callback (stream, status, event)
   type( c_ptr ) :: event
   integer(kind=omp_event_handle_kind) :: f_event
    call C_F_POINTER (event, f_event)
    call omp_fulfill_event( f_event )
end subroutine callback
```

1. A: launch FFT, add call to *callback* in stream where FFT is running
2. B waits as dependent on A, C executes asynchronously
3. After FFT, function *callback* is called and event fulfilled
4. A completes allowing B to run

Support for `DETACH` not yet available

Summary (I)

- Developed a new algorithm for Summit capable of 18432^3 problem size (currently world's largest DNS), presented as best student paper finalist at SC19
  — optimized strided data copies and all-to-all communication
  — 3X faster than pencil decomposition CPU code, 4.5X for 12288^3
- Successfully developed particle tracking capabilities using the batched asynchronous algorithm capable of 18432^3 with 1.5 billion particles
- Steps to overcome challenges in porting code to OpenMP; pending compiler support
  — `DETACH` for async. execution of GPU library calls with OpenMP tasks

Developed an algorithm to enable extreme-scale simulations using advanced heterogeneous architectures

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Intermittency using high resolution simulations

- Extreme events characterizing intermittency in high R_λ turbulence poses stringent resolution requirements in both time and space (Yeung *et al.* 2018)
- High spatial resolution: capable of capturing larger local gradients
- Long simulations at high resolution are impossible, computational resources limited
- Limitations of sampling and independence: obscure benefits of increased resolution
- Multiple Resolution Independent Simulation (MRIS) approach
  — Average over multiple short independent simulations (Yeung *et al.* 2020)
- Intermittency through statistics of energy dissipation and enstrophy
  — Refined Similarity Theory (Kolmogorov 1962): moments of 3D local averages

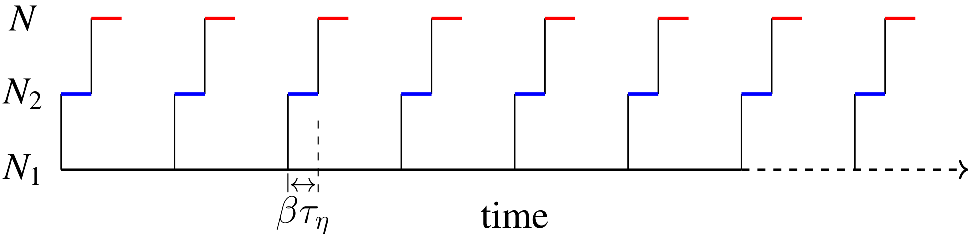
Multiple-Resolution Independent Simulations

Small scale processes in stationary isotropic turbulence (Yeung *et al* 2018, 2020)

- Have short time scales: take samples from short simulations
- Adjust to new resolution quickly (within 1-2 Kolmogorov time scales)

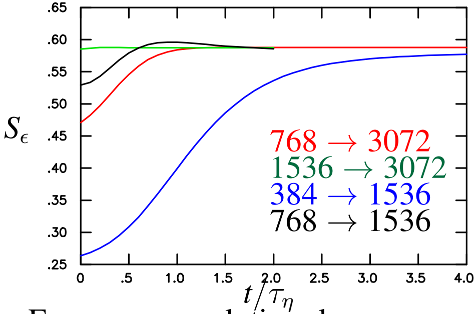
MRIS approach: replace long simulation by multiple short simulations

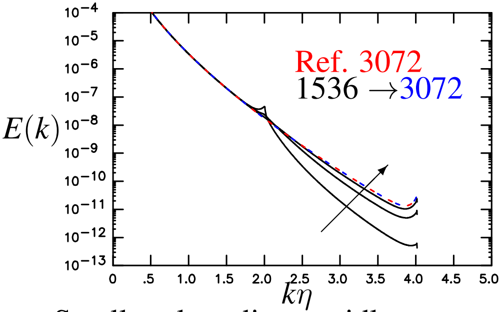
- Initial snapshots at lower resolution (N_1), spaced out in time for better independence
- M segments of grid refinement ($N_1 \to N$ or $N_1 \to N_2 \to N$), each $t \sim \beta\tau_\eta$ ($\beta \sim$1-2)
- Most appealing when ratio T_E/τ_η is large (i.e. at high Reynolds numbers)



Validation of MRIS

- Remove high wavenumber modes in N^3 simulation; truncated field of resolution N_1^3
- Run simulation at N^3 resolution, starting with N_1^3; check if original results recovered
- Recovery time increases as N/N_1; Simulations at intermediate resolution, N_2^3
- Study skewness of dissipation (S_ϵ) and Energy spectrum ($E(k)$) in $R_\lambda \sim 390$





- From poor resolution: longer recovery
- Two refinements: short recovery
- Small scales adjust rapidly

Overview of Simulations

- First segment $C = 0.3$, from snapshots in $C = 0.6$ simulation
- Two successive grid refinements until $k_{max}\eta$ reaches 4.2-4.5 ($k_{max} = \sqrt{2}N/3$)

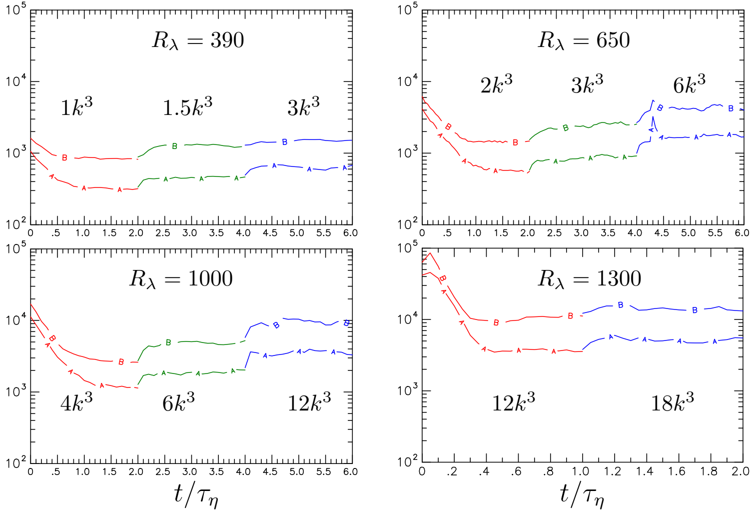
- R_λ 1300 using new code
  — First segment: reduces C and grid refinement starting from 8192^3
  — Also shorter, $\beta = 1$
- Second-order moments
  — increase with R_λ
  — $k_{max}\eta \geq 2.1$, weak dependence
- Ω more intermittent than ϵ

R_λ	N	$k_{max}\eta$	β	M	$\langle\epsilon^2\rangle/\langle\epsilon\rangle^2$	$\langle\Omega^2\rangle/\langle\Omega\rangle^2$
390	1024	1.4	2	22	3.869	7.665
390	1536	2.1	2	22	4.034	7.938
390	3072	4.2	2	22	4.074	7.969
650	2048	1.4	2	15	4.357	8.718
650	3072	2.1	2	15	4.575	9.133
650	6144	4.2	2	15	4.664	9.214
1000	4096	1.4	2	10	4.949	9.901
1000	6144	2.1	2	10	5.250	10.556
1000	12288	4.2	2	10	5.381	10.745
1300	12288	3.0	1	10	6.103	12.238
1300	18432	4.5	1	10	6.142	12.288

Evolution of extreme events

- Drop in first half of first segment (Yeung *e*t al. 2018)
- Steeper drop for R_λ 1300 — strong suppression of alias: better resolution in $\mathbf{x}$ & t
- Grid refinement: jump in peak values as larger $|\partial u_i/\partial x_j|$ captured
- Ω more intermittent than ϵ

Ensemble averaged peak values of A:$\epsilon/\langle\epsilon\rangle$ & B:$\Omega/\langle\Omega\rangle$



3D local averages of dissipation and enstrophy

- Central issue in refined scale similarity (Kolmogorov 1962)

$$\epsilon_r = \frac{1}{Vol} \int_r \epsilon(\mathbf{x} + \mathbf{r}) \, d\mathbf{r} \; .$$

- Moments of ϵ_r show power-law dependencies ($\langle \epsilon_r^q \rangle \propto r^{\zeta_q}$), in inertial range?
- Compute the exponents from logarithmic local slopes, $\zeta_q = d \log(\langle \epsilon_r^q \rangle / \langle \epsilon \rangle^q) / d(r/\eta)$
- Conditional moments to understand how ϵ and Ω scale with each other

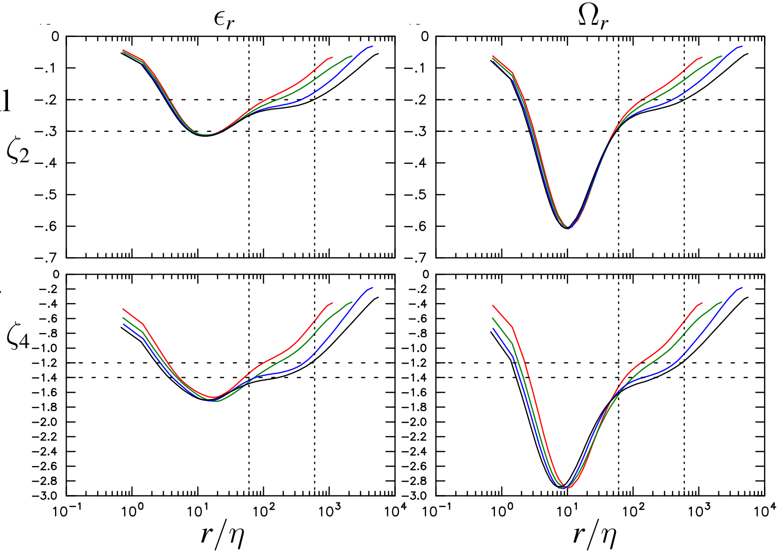
$$\langle \Omega_r^q | \epsilon_r \rangle / \langle \Omega \rangle^q \qquad ; \qquad \langle \epsilon_r^q | \Omega_r \rangle / \langle \epsilon \rangle^q$$

- Computationally challenging: 3D local averages relatively rare (Iyer *e*t al. 2015)

Local averages key to refined similarity accounting for intermittency

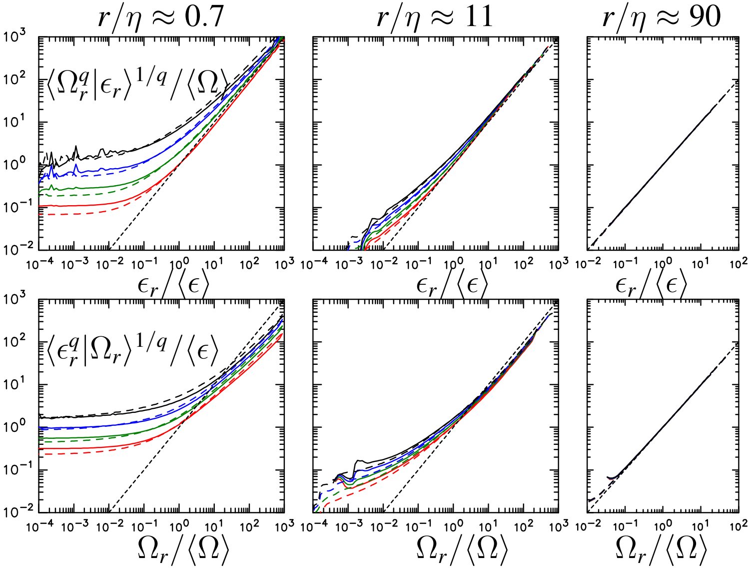
Slope of 2^{nd} & 4^{th} moments of ϵ_r & Ω_r: R_λ 390, 650, 1000, 1300

- Leveling off at small r/η ($\zeta_q \to 0$): small scales well resolved
- Plateau in inertial range, $60 < r/\eta < 600$, as $R_\lambda \uparrow$
- $\zeta_2 \approx 0.23$ for both ϵ_r & Ω_r
- Ω_r more intermittent than ϵ_r in dissipation range — $r/\eta \approx 10$, $\zeta_{q,\Omega} < \zeta_{q,\epsilon}$
- Similar in inertial range: homogeneity



Conditional moments: $q = 1, 2, 3, 4$; R_λ 390 (solid), 1000 (dash)

- Weak R_λ effects
- High $\epsilon_r \rightarrow$ high Ω_r
- High $\Omega_r \rightarrow$ slightly lower ϵ_r
- Low Ω_r or ϵ_r, scale independently
- ϵ_r & Ω_r scale together in inertial range



Summary (II)

- Developed a Multiple Resolution Independent Simulation approach: production results at high resolution and Reynolds number from extreme-scale simulations
- The approach was validated for use in studies of small-scales
- MRIS successfully used to generate high fidelity results up to R_λ 1300
- Power-law behavior in moments of local averages especially at high R_λ

Use advanced algorithms & compute platforms for high-resolution studies of fine-scale intermittency

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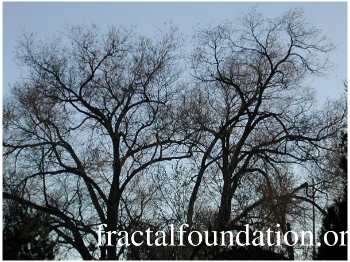
What are multifractals?

- Self-similar energy cascade: energy dissipation unevenly distributed among small-scales
  — multifractal framework well-suited for such processes
- Fractals: "objects" that display self-similar properties over wide range of scales
- A characteristic dimension: "fractal dimension"
  — unlike Euclidean dimensions need not be integer



- Dynamics of complex processes (turbulence): continuous spectrum of dimensions called the multifractal spectrum
- Commonly studied "fractal object": energy dissipation rate (Sreenivasan *et al.* 1986)
- High resolution & Reynolds number DNS data to compute multifractal spectrum

Computing multifractal spectrum from DNS data

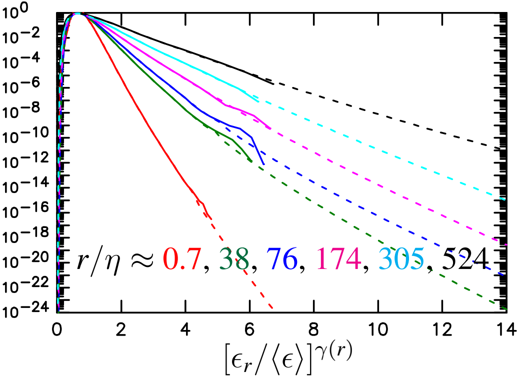
- For "multiplicative processes", based on conservation laws (Meneveau *et al.* 1991)
$$F(r,q) = [\sum (E_r/E_0)^q]^{(1/(q-1))} \sim (r/L)^{D_q}$$
summation is over all boxes of size r, q is the order, $E_r = \epsilon_r r^3$ is the total energy dissipation over a volume of size r^3 and D_q is generalized dimension.
- Local averages of energy dissipation: $F(r,q) = (r/L_0)^3 [\langle \epsilon_r^q \rangle / \langle \epsilon \rangle^q]^{(1/(q-1))}$
- Multifractal spectrum ($f(\alpha)$) using generalized dimensions: $f(\alpha) = q\alpha - (q-1)D_q$
- α characterizes strength of near-singularities: $\alpha(q) = \frac{d}{dq}[(q-1)D_q]$
- Full definition of energy dissipation (all nine velocity gradients) and 3D averages — past lab experiments used 1D surrogates and Taylors frozen-flow hypothesis
- High-resolution ($k_{max}\eta$ 4.2-4.5) DNS data from MRIS: $R_\lambda \sim 390, 650, 1000$ & 1300

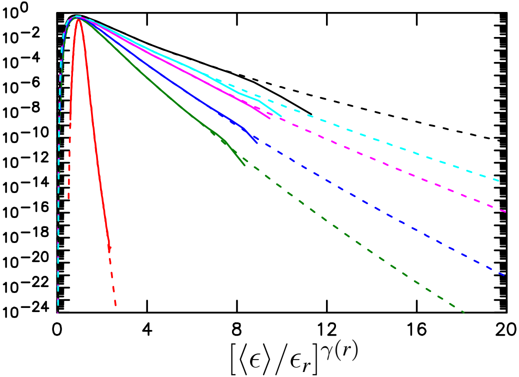
Extrapolation of PDF tails at $R_\lambda \sim 1300$

- Moments of $\epsilon_r/\langle\epsilon\rangle$ crucial to compute $f(\alpha)$
- High positive and negative moments: PDF tails show lack of convergence
- Extrapolate PDF tails using stretched exponentials (SE):

$$p(\epsilon_r/\langle\epsilon\rangle) \sim \exp[-a(r)(\epsilon_r/\langle\epsilon\rangle)^{\gamma(r)} + b(r)]$$

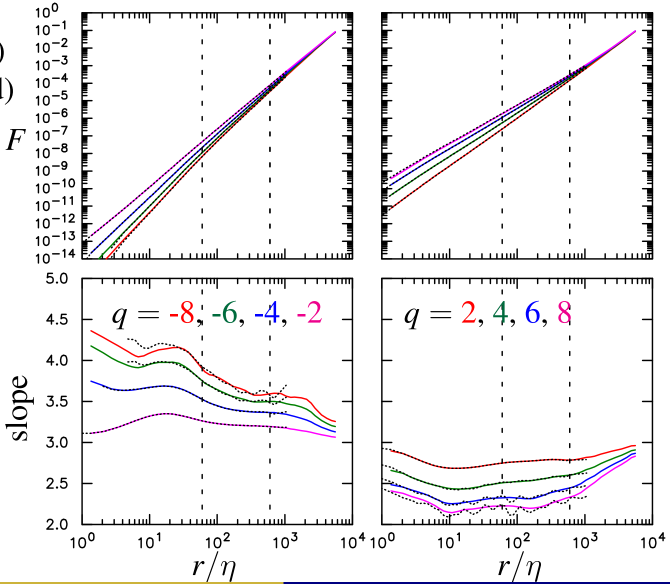
- Extrapolation only for $r/\eta < 1100$; reliable curve fits difficult for higher r/η



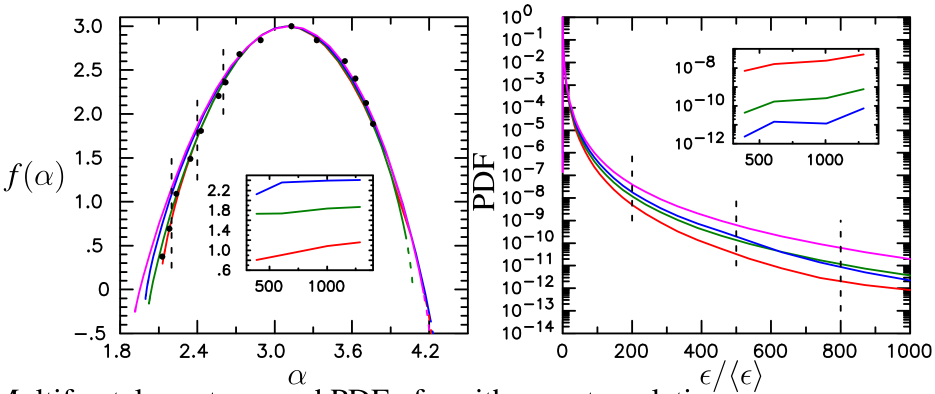


Multifractal moments and local slopes from data at $R_\lambda \sim 1300$

- Moments from actual PDFs (solid) and SE-extrapolated PDFs (dashed)
- Power-law: constant local slope
- Variability of slopes in $60 < r/\eta < 600$ less than 10%
- Not clear for high -ve orders
- Scaling range varies with q
- Good agreement b/w actual PDFs and SE-extrapolation
- Some noise in extrapolated data; use least squares fit for D_q



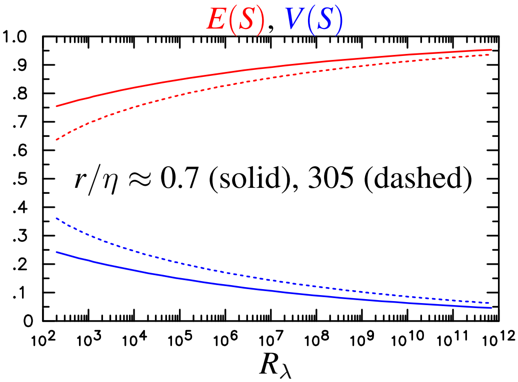
Robustness multifractal spectrum: $R_\lambda \sim$ 390, 650, 1000, 1300



- Multifractal spectrum and PDF of ϵ with no extrapolation
- For R_λ dependence: relative variability for fixed α and $\epsilon/\langle\epsilon\rangle$
- $\alpha = 2.2$: variability b/w R_λ 390 & 1300 is 30%, but b/w 1000 & 1300 is 6%
- $\epsilon_r/\langle\epsilon\rangle = 800$: variability b/w R_λ 390 & 1300 is 97%, while b/w 1000 & 1300 is 84%
- $f(\alpha)$ vs α agrees well with data from Meneveau *et al.* 1991 (used 1D surrogates)

Energy dissipation and volume occupied by near-singularities

- "Near-singularities" defined by a set S
- Energy dissipation contribution
  $$E(s) = \int_{\alpha\in S}(r/L_0)^{\alpha-f(\alpha)}d\alpha$$
- Volume occupied
  $$V(S) = \int_{\alpha\in S}(r/L_0)^{3-f(\alpha)}d\alpha$$
  Sreenivasan *et al.* 1988
- Use multifractal spectrum at $R_\lambda \sim 1300$ to compute the quantities
- Singularities corresponding to high dissipation, $\alpha < 3$



- Most of ϵ contained in singularities occupying small volume especially at high R_λ
- Approach to asymptotic values of 0 and 1 slow with R_λ, not for any practical case

Summary (III)

- Multifractal perspective, full definition of ϵ (no approximations), 3D local averages
- Stretched exponential extrapolation of PDF tails for ϵ_r over wide range of scale sizes
- Multifractal spectrum robust to changes in R_λ and use 1D averages and approximations like 1D surrogates
- Near-singularities corresponding to $\alpha < 3$ (high dissipation) contribute more to total energy dissipation while occupying even smaller volumes, as R_λ increases

Analysis of energy dissipation rate from a multifractal perspective using high resolution DNS data at high Reynolds number

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- Introduction
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Intermittency in passive scalars

- Unity or higher *Sc* scalar: strong intermittency than velocity (Gotoh & Yeung 2013)
- Extreme values of scalar dissipation rate ($\chi \equiv 2D|\nabla\phi|^2$): large scalar gradients — difficult to capture; need high resolution simulations
- Additional wallclock time to simulate scalars: long simulations more difficult
- MRIS approach for high-reslolutions studies of passive scalar intermittency
- Two scalars of $Sc = 1$ and $Sc = 0.125$: relevant in gaseous combustion
- Average results of scalars driven by uniform mean gradient in different directions
- Single point statistics of scalar dissipation and comparison to energy dissipation
- Refined similarity theory: Local averages of scalar dissipation rate

Overview of simulations

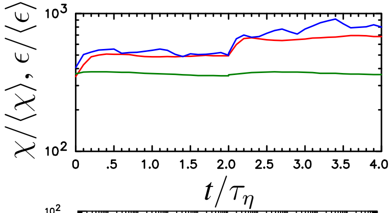
R_λ	N	$k_{max}\eta$	Sc		β	M	$\langle\epsilon^2\rangle/\langle\epsilon\rangle^2$	$\langle\chi^2\rangle/\langle\chi\rangle^2$		$\mu_3(\nabla_{\|\|}\phi)$	
			Sc_1	Sc_2				Sc_1	Sc_2	Sc_1	Sc_2
390	1024	1.4	1	0.125	2	11	4.19	13.42	11.99	1.24	1.85
390	1536	2.1	1	0.125	2	11	4.35	15.32	11.95	1.36	1.85
390	3072	4.2	1	0.125	2	11	4.39	15.77	11.90	1.38	1.84
650	2048	1.4	1	-	2	21	4.62	16.90	-	1.19	-
650	3072	2.1	1	-	2	21	4.88	19.70	-	1.32	-
650	6144	4.2	1	-	1	21	4.98	20.52	-	1.35	-

- Second-order moment, $\chi > \epsilon$, more intermittent (Overholt *et al.* 1996)
- $\langle\epsilon^2\rangle/\langle\epsilon\rangle^2$ unchanged as resolution improved, $k_{max}\eta \sim 4.2$ sufficient for second order
- But for $Sc = 1$, $\langle\chi^2\rangle/\langle\chi\rangle^2$ could benefit from higher resolution, especially at high R_λ
- Higher $k_{max}\eta$ and $Sc \rightarrow$ larger $\mu_3(\nabla_{\|\|}\phi)$; Return to local isotropy with R_λ is slow

Single point statistics of scalar and energy dissipation

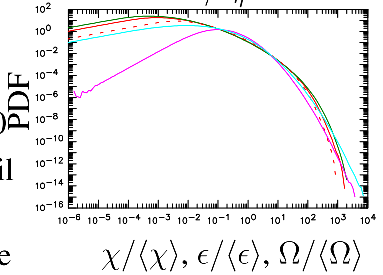
Peak $\epsilon/\langle\epsilon\rangle$ and $\chi/\langle\chi\rangle$ ($Sc =$1, 0.125) at $R_\lambda \sim 390$

- Grid refinement at $t = 0$ and $2\tau_\eta$
- Adjusts to higher resolution by $t = 0.5\tau_\eta$
- Higher peak values as resolution increased
  — larger magnitude gradients captured
  — $Sc = 0.125$ already well resolved



PDF of $\epsilon/\langle\epsilon\rangle$, $\chi/\langle\chi\rangle$ at R_λ 390 and 650, $k_{max}\eta$ 4.2

- Red dashed: $Sc = 0.125$, ϵ (magenta), Ω (cyan) at R_λ 650
- Moderate χ ($Sc = 1$) more probable than ϵ but ϵ wider tail
  — high order moments of ϵ catch up to χ
- Small sample values, power-law behavior; gradients close to Gaussian (Yeung *et al.* 2012)

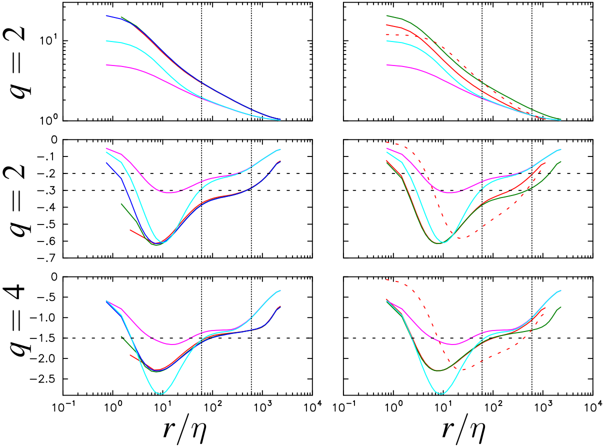


Scaling of moments of local averages of χ_r, ϵ_r and Ω_r

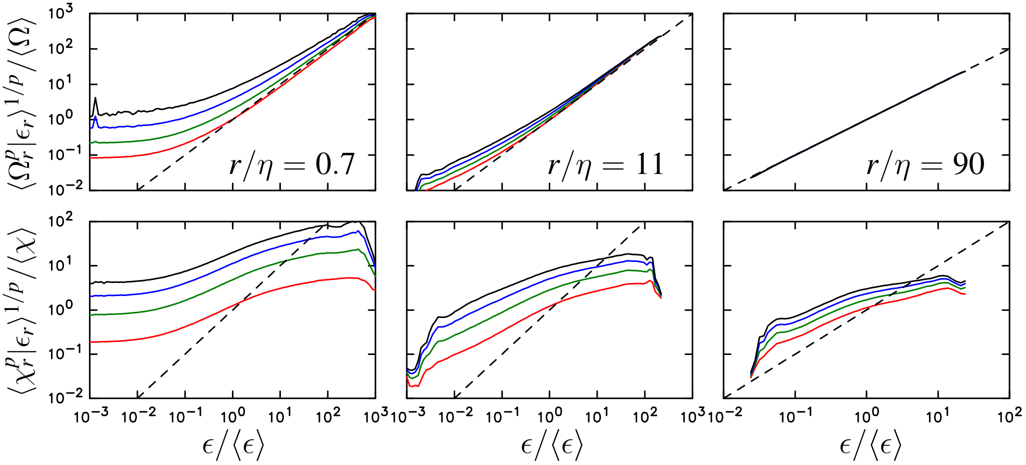
- Plateau observed for ζ_q in inertial range — $Sc = 0.125$ (dashed), no definitive inertial-convective range
- Clearer: high R_λ, low q & for χ than ϵ
- Local slope at small r/η: ϵ, Ω at $p = 2$ better resolved
- Larger ζ_p for χ at $Sc = 1$: stronger inertial-convective range intermittency

χ_r: $k_{max}\eta \sim 1.4, 2.1, 4.2$, $R_\lambda \sim 650$ | χ_r: $R_\lambda \sim 390, 650$, $k_{max}\eta \sim 4.2$

ϵ, Ω at $k_{max}\eta \sim 4.2$, $R_\lambda \sim 650$



Conditional moments of Ω_r, χ_r given ϵ_r: R_λ 650, $p = 1, 2, 3, 4$



- Extreme Ω and ϵ scale similarly at all r/η; perfect scaling in inertial range
- Extreme ϵ not accompanied by extreme χ; better scaling in inertial-convective range

Summary (IV)

- MRIS technique applied successfully for studies of passive scalar intermittency
- PDFs showed moderately large χ more probable than ϵ, low to moderate order moments dominated by χ, but ϵ might catch up at higher orders
- Skewness of scalar gradients $\|$ to mean gradient: strong departure from local isotropy with a slow return as R_λ increases
- Power-law behavior in moments of local averages especially at high R_λ
- Small-scale of the scalar field: stricter resolution requirements than velocity field
- Peak values of scalar & energy dissipation do not scale with each other unlike ϵ & Ω

MRIS approach used to study small-scales of passive scalars and how they compare to velocity field

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Introduction

- Stratified flows with two active scalars of different molecular diffusivities: focus on differential diffusion effects (Turner 1974; Schmitt 1994)
- Most common in ocean with temperature and salinity (high Sc), but also seen in astrophysical flows with very low Sc (Garaud 2018)
- Stable stratification: oscillatory behavior and suppressed turbulence
- Unstable: strong growth of turbulence leading to strict resolution requirements
- Flow is non-stationary and anisotropic
- Stratification strength, ratio of buoyancy to turbulence time scales
  — Froude number: $F_i = T_i/(L/u')$, where $T_i = 2\pi/(gc_i|d\Phi_i/dz|)^{1/2}$
  — Low F_i or large magnitude of $d\Phi_i/dz$: strong stratification

Preliminary simulations

- Naturally decaying isotropic turbulence as initial conditions

No.	Problem size	Froude No. Sc=0.1	Froude No. Sc=0.01	Mean Gradient Sc=0.1	Mean Gradient Sc=0.01	R_{λ_0}	R_{λ_n}	$k_{max}\eta_0$	$k_{max}\eta_n$
S1	4096×512^2	1	1.1	93	-77	22	89	1.64	0.88
S2	16384×2048^2	2	2	82	-82	64	129	1.29	1.41
S3	16384×2048^2	1	2	328	-82	64	166	1.29	3.83
S4	16384×2048^2	1	1	328	-328	64	143	1.29	0.70

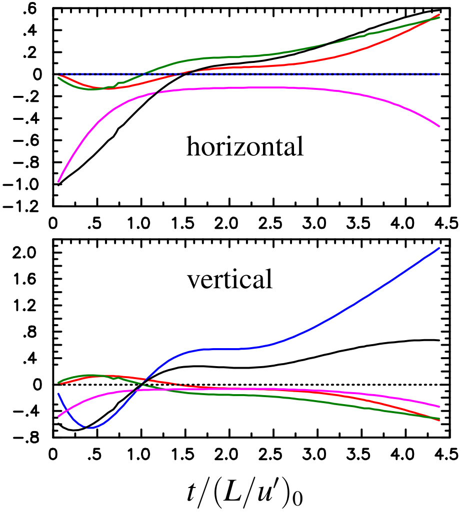
- S1 with & without diagonalized scheme agree well, shows turbulence blows up
- S4 shows small scales become poorly resolved, need progressive grid refinement
- Long-time behavior for unstable stratification: buoyancy contributions raise questions about validity of Boussinesq approximation

Reynolds stress budget: unstable stratification

- Different terms in the Reynolds stress budget

$$\frac{d\langle u_i u_j\rangle}{dt} = \langle 2p^{(s)} s_{ij}\rangle + \langle 2p^{(b)} s_{ij}\rangle - (\langle \rho' u_i \delta_{j3}\rangle + \langle \rho' u_j \delta_{i3}\rangle) - \langle \epsilon_{ij}\rangle$$

- Slow & buoyancy pressure strain, re-distributive
- Buoyancy flux non-zero along vertical
- At early time, buoyancy flux is negative — slow pressure transfers energy from horizontal to vertical components
- At later time, buoyancy flux is strong production — inter-component energy transfer reverses
- Buoyancy press. strain similar to slow pressure
- Growth in K supported by positive rate of change at later times



Summary (V)

Perform new simulations vertically elongated and flattened domains

- Unstable stratification: vertically elongated domains with finer grid resolution
- Stable stratification: flattened domains

Analysis of simulations and understanding anisotropy development

- Reynolds stress budget, anisotropy at different scale sizes, visualization of flow
- Assess validity of Boussinesq approx. especially at later times under unstable cases
- Study differential diffusion effects with two active scalars of opposing effects

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Summary and contributions (I)

GPU acceleration of extreme scale pseudo-spectral simulations of turbulence using asynchronism

- A new batched asynchronous algorithm enabling world-leading grid resolution 18432^3 (more than 6 trillion grid points)
- Further extended to simulate passive, active scalars and Lagrangian fluid particles
- Portability challenges addressed: use of advanced OpenMP 5.0 features for correct interoperability between Numerical libraries and OpenMP tasks
- Code development & optimization in progress: target 32768^3 on Frontier, early 2022
- Paper at supercomputing 2019 and best student paper finalist
- Paper on OpenMP work in Parallel Computing Journal (2021, accepted) & in Proc. 17th International Workshop on OpenMP (IWOMP, 2021)
- At leading workshops & conferences, eg., P3HPC, OpenPower, DoE PPP, APS 2018

Summary and contributions (II)

Advancing understanding of turbulence through extreme-scale computation: intermittency and simulations at large problem sizes

- Developed new approach, "Multiple Resolution Independent Simulations" (MRIS): alternate to long simulations impossible due to limited computational resource
- Improved statistical sampling and independence among snapshots
- Studies of intermittency: flows of $R_\lambda \sim 1300$ & $k_{max}\eta \sim 4.5$ using 18432^3 grid points
- Power-law scaling over wide range of scales for both energy dissipation & enstrophy
- Conditional moments: high ϵ scale with Ω but opposite not always true
- Invited paper, Yeung & Ravikumar, *Phys Rev. Fluids*, 2020
- Invited talk at APS 2019 and presentations at other conferences

Summary and contributions (III)

Extreme dissipation and its multifractal nature at high Reynolds numbers

- Energy dissipation from multifractal viewpoint: geometric perspective of small-scale
- High-resolution DNS data (up to $k_{max}\eta \sim 4.5$) from MRIS work up to $R_\lambda \sim 1300$
- Energy dissipation using all nine velocity gradients and 3D averages
- Stretched exponential to model behavior of PDF tails for ϵ_r over wide range of scales
- Generalized dimensions & multifractal spectrum computed
- Near-singularities: Small volumes contain most dissipation, especially high R_λ
- Manuscript under preparation

Summary and contributions (IV)

High resolution studies of intermittency in scalar dissipation rates (χ)

- MRIS for high-resolution study of passive scalars subject to uniform mean gradient
- Stricter resolution requirements for small-scales of scalar compared to velocity
- Moderately large scalar dissipation more probable than energy dissipation, low-order moments high for χ but ϵ might catch up at higher orders
- Power-law scaling: moments of local averages of χ in inertial-convective range
- Conditional moments of χ & ϵ: does not scale with each other
- Presented at APS 2020

Summary and contributions (V)

Active scalar turbulence and double diffusive phenomena

- Preliminary study of stratified turbulence with two active scalars
- Anisotropy development in Reynolds stress tensor for stable & unstable stratification
- Presented at APS 2020

Future considerations

Some ideas to continue and extend the work in this thesis

- Using GPU-Direct technology for global transposes
- Numerical simulations of Stoke's particles
- Passive scalar simulations at high Schmidt number using GPUs
- Studies of intermittency at higher Reynolds numbers via extreme scale computing
- Multifractal analysis of passive scalars
- Refined similarity theory of passive scalars at high resolution and Reynolds number
- Resolution effects and Boussinesq approximation in active scalar simulations
- Differential diffusion effects in stratified flows