Filtered Density Function (for LES) and the Potentials for its Quantum Computation

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Outline

1. LES via FDF.

2. Towards Petascale FDF Simualtion.

3. Quantum Speed-up?

Filtered (Mass) Density Function

- **PDF at the subgrid scale (SGS).**
- **Scalar-FDF: SGS chemical reaction effects in a closed form.**
- **Velocity-Scalar FDF: SGS convection in a closed form.**
- **More parameters FDF: more complex physics.**

$$\langle Q(x,t)\rangle_l = \int_{-\infty}^{+\infty} Q(x',t)\, G(x',x)\, dx' \qquad \langle Q(x,t)\rangle_L = \frac{\langle \rho Q\rangle_l}{\langle \rho\rangle_l}$$

$$\langle \rho(x,t)\rangle_l \langle Q(x,t)\rangle_L = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \langle Q(x,t)\,|V,\psi,\theta,\eta\rangle_l\, F_L(V,\psi,\theta,\eta,x;t)\, dV d\psi d\theta d\eta$$

Low Speed Combustion

$$\frac{\partial \langle \rho \rangle_l}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_j \rangle_L}{\partial x_j} = 0$$

$$\frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_j \rangle_L \langle u_i \rangle_L}{\partial x_j} = -\frac{\partial \langle p \rangle_l}{\partial x_i} + \frac{\partial \breve{\tau}_{ij}}{\partial x_j} - \frac{\partial \langle \rho \rangle_l \tau_L \;\; u_i, u_j}{\partial x_j}$$

$$\frac{\partial \langle \rho \rangle_l \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_j \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_j} = -\frac{\partial \breve{J}_j^\alpha}{\partial x_j} - \frac{\partial \langle \rho \rangle_l \tau_L \;\; \phi_\alpha, u_j}{\partial x_j} + \langle \rho S_\alpha \rangle_l$$

SGS unclosed terms:

$$\tau_L \;\; u_i, u_j \;\; = \langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L \qquad \tau_L \;\; \phi_\alpha, u_j \;\; = \langle u_j \phi_\alpha \rangle_L - \langle u_j \rangle_L \langle \phi_\alpha \rangle_L$$

$$\langle \rho S_\alpha \rangle_l = \langle \rho \rangle_l \langle S_\alpha \rangle_L$$

VS-FDF

Fine Grain Density:

$$\zeta\left[V,\psi;u(x,t),\phi(x,t)\right]=\left(\prod_{k=1}^{3}\delta\left[V_k-u_k(x,t)\right]\right)\times\left(\prod_{\alpha=1}^{N_s}\delta\left[\psi_\alpha-\phi_\alpha(x,t)\right]\right)$$

FDF:

$$F_L(V,\psi,x;t)\equiv\int_{-\infty}^{+\infty}\rho(x',t)\,\zeta\left[V,\psi;u(x',t),\phi(x',t)\right]G(x'-x)\,dx'$$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}F_L(V,\psi,x;t)\,dV\,d\psi=\left\langle\rho\right\rangle_l$$

High Speed Turbulence

$$\frac{\partial\left\langle \rho\right\rangle_l}{\partial t}+\frac{\partial\left\langle \rho\right\rangle_l\left\langle u_j\right\rangle_L}{\partial x_j}=0$$

$$\frac{\partial\left\langle \rho\right\rangle_l\left\langle u_i\right\rangle_L}{\partial t}+\frac{\partial\left\langle \rho\right\rangle_l\left\langle u_j\right\rangle_L\left\langle u_i\right\rangle_L}{\partial x_j}=-\frac{\partial\left\langle p\right\rangle_l}{\partial x_i}+\frac{\partial\breve{\tau}_{ij}}{\partial x_j}-\frac{\partial\left\langle \rho\right\rangle_l\tau_L\;\;u_i,u_j}{\partial x_j}$$

$$\frac{\partial\left\langle \rho\right\rangle_l\left\langle e\right\rangle_L}{\partial t}+\frac{\partial\left\langle \rho\right\rangle_l\left\langle u_j\right\rangle_L\left\langle e\right\rangle_L}{\partial x_j}=-\frac{\partial\breve{q}_j}{\partial x_j}-\frac{\partial\left\langle \rho\right\rangle_l\tau_L\;\;e,u_j}{\partial x_j}$$

$$+\varepsilon+\breve{\tau}_{ij}\frac{\partial\left\langle u_i\right\rangle_L}{\partial x_j}-\Pi_d-\left\langle p\right\rangle_l\frac{\partial\left\langle u_i\right\rangle_L}{\partial x_i}$$

$$\frac{\partial\left\langle \rho\right\rangle_l\left\langle \phi_\alpha\right\rangle_L}{\partial t}+\frac{\partial\left\langle \rho\right\rangle_l\left\langle u_j\right\rangle_L\left\langle \phi_\alpha\right\rangle_L}{\partial x_j}=-\frac{\partial\breve{J}_j^\alpha}{\partial x_j}-\frac{\partial\left\langle \rho\right\rangle_l\tau_L\;\;\phi_\alpha,u_j}{\partial x_j}$$

EPVS-FDF

Fine Grain Density:

$$\zeta\left[V,\psi,\theta,\eta;u(x,t),\phi(x,t),e(x,t),p(x,t)\right]=$$

$$\left(\prod_{k=1}^{3}\delta\left[V_k-u_k(x,t)\right]\right)\times\left(\prod_{\alpha=1}^{N_s}\delta\left[\psi_\alpha-\phi_\alpha(x,t)\right]\right)\times\delta\left[\theta-e(x,t)\right]\times\delta\left[\eta-p(x,t)\right]$$

FDF:

$$F_L(V,\psi,\theta,\eta,x;t)\equiv\int_{-\infty}^{+\infty}\rho(x',t)\,\zeta\left[V,\psi,\theta,\eta;u(x',t),\phi(x',t),e(x',t),p(x',t)\right]G(x'-x)\,dx'$$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}F_L(V,\psi,\theta,\eta,x;t)\,dVd\psi d\theta d\eta=\langle\rho\rangle_l$$

Exact VS-FDF Transport

$$\frac{\partial F_L}{\partial t} + \frac{\partial V_j F_L}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\mu \frac{\partial \; F_L / \rho \;\; \psi}{\partial x_j}\right] - \frac{\partial}{\partial \psi_\alpha}\left[S_\alpha \;\; \psi \;\; F_L\right]$$

$$+\frac{\partial}{\partial V_i}\left[\frac{1}{\rho \;\; \psi}\left\langle \frac{\partial p}{\partial x_i}\middle| V, \psi \right\rangle F_L\right] - \frac{\partial^2}{\partial V_i \partial V_j}\left[\frac{\mu}{\rho \;\; \psi}\left\langle \frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}\middle| V, \psi \right\rangle F_L\right]$$

$$-\frac{\partial}{\partial V_i}\left[\frac{1}{\rho \;\; \psi}\left\langle \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_j}{\partial x_i}\right)\middle| V, \psi \right\rangle F_L\right] + \frac{\partial}{\partial V_i}\left[\frac{1}{\rho \;\; \psi}\left\langle \frac{\partial}{\partial x_i}\left(\frac{2}{3}\mu \frac{\partial u_j}{\partial x_j}\right)\middle| V, \psi \right\rangle F_L\right]$$

$$-2\frac{\partial^2}{\partial V_i \partial \psi_\alpha}\left[\frac{\mu}{\rho \; \psi}\left\langle \frac{\partial u_i}{\partial x_j}\frac{\partial \phi_\alpha}{\partial x_j}\middle| V, \psi \right\rangle F_L\right] - \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta}\left[\frac{\mu}{\rho \; \psi}\left\langle \frac{\partial \phi_\alpha}{\partial x_j}\frac{\partial \phi_\beta}{\partial x_j}\middle| V, \psi \right\rangle F_L\right]$$

Langevin Descriptor

- Lagrangian vector variables

$$Z\ \ t\ \ = \left[X^{+}, U^{+}, \phi^{+}, E^{+}, P^{+} \right]$$

- Diffusion process

$$dZ\ \ t\ \ = D\ \ Z\ \ t\ \ ,t\ \ dt + E\ \ Z\ \ t\ \ ,t\ \ dW\ \ t$$

- Compare the corresponding Fokker-Planck equation with FDF

$$D = \ldots \quad , \quad E = \ldots$$

Fokker-Planck

$$
\begin{aligned}
\frac{\partial F_L}{\partial t} + \frac{\partial V_i F_L}{\partial x_i} &= \frac{1}{\langle\rho\rangle_l}\frac{\partial \langle p\rangle_l}{\partial x_i}\frac{\partial F_L}{\partial V_i} - \frac{2}{\langle\rho\rangle_l}\frac{\partial}{\partial x_j}\left(\mu \frac{\partial \langle u_i\rangle_L}{\partial x_j}\right)\frac{\partial F_L}{\partial V_i} - \frac{1}{\langle\rho\rangle_l}\frac{\partial}{\partial x_j}\left(\mu \frac{\partial \langle u_j\rangle_L}{\partial x_i}\right)\frac{\partial F_L}{\partial V_i} \\
&+ \frac{2}{3}\frac{1}{\langle\rho\rangle_l}\frac{\partial}{\partial x_i}\left(\mu \frac{\partial \langle u_j\rangle_L}{\partial x_j}\right)\frac{\partial F_L}{\partial V_i} - \frac{\partial\, G_{ij}\left(V_j - \langle u_j\rangle_L\right) F_L}{\partial V_i} + \frac{\partial}{\partial x_i}\left(\mu \frac{\partial \left(F_L / \langle\rho\rangle_l\right)}{\partial x_i}\right) \\
&+ \frac{\partial}{\partial x_i}\left(\frac{2\mu}{\langle\rho\rangle_l}\frac{\partial \langle u_j\rangle}{\partial x_i}\frac{\partial F_L}{\partial V_j}\right) + \frac{\mu}{\langle\rho\rangle}\frac{\partial \langle u_k\rangle}{\partial x_j}\frac{\partial \langle u_i\rangle}{\partial x_j}\frac{\partial^2 F_L}{\partial V_k \partial V_i} + \frac{1}{2}C_0\frac{\varepsilon}{\langle\rho\rangle_l}\frac{\partial^2 F_L}{\partial V_i \partial V_i} \\
&+ C_\phi \omega \frac{\partial \left[\left(\psi_\alpha - \langle\phi_\alpha\rangle_L\right) F_L\right]}{\partial \psi_\alpha} + \frac{C_e}{\gamma}\omega \frac{\partial \left[\left(\theta - \langle e\rangle_L\right) F_L\right]}{\partial \theta} - \frac{\gamma - 1}{\gamma}\left(\varepsilon + \breve{\tau}_{ij}\frac{\partial \langle u_i\rangle_L}{\partial x_j}\right)\frac{\partial}{\partial \theta}\left(\frac{\theta}{\eta}F_L\right) \\
&- \frac{\gamma - 1}{\gamma}\frac{\partial \left(\theta A F_L\right)}{\partial \theta} + \frac{\gamma - 1}{\gamma^2}\frac{\partial \left(\theta B^2 F_L\right)}{\partial \theta} - \frac{\partial \left(\eta A F_L\right)}{\partial \eta} + \frac{1}{2}\frac{\left(\gamma - 1\right)^2}{\gamma^2}\frac{\partial^2 \left(\theta^2 B^2 F_L\right)}{\partial \theta \partial \theta} \\
&+ \frac{\gamma - 1}{\gamma}\frac{\partial^2 \left(\theta \eta B^2 F_L\right)}{\partial \theta \partial \eta} + \frac{1}{2}\frac{\partial^2 \left(\eta^2 B^2 F_L\right)}{\partial \eta \partial \eta}
\end{aligned}
$$

Modeled 2nd Order SGS Equations

$$\frac{\partial \langle \rho \rangle_l \tau_L\ \ u_i, u_j}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_k \rangle_L \tau_L\ \ u_i, u_j}{\partial x_k} = \langle \rho \rangle_l P_{ij} - \frac{\partial}{\partial x_k}\left(\langle \rho \rangle_l \tau_L\ \ u_k, u_i, u_j\ \ - \mu \frac{\partial \tau_L\ \ u_i, u_j}{\partial x_k} \right)$$

$$+ G_{jk} \langle \rho \rangle_l \tau_L\ \ u_k, u_i\ \ + G_{ik} \langle \rho \rangle_l \tau_L\ \ u_k, u_j\ \ + C_0 \varepsilon \delta_{ij}$$

$$\frac{\partial \langle \rho \rangle_l \tau_L\ \ \phi_\alpha, \phi_\beta}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_k \rangle_L \tau_L\ \ \phi_\alpha, \phi_\beta}{\partial x_k} = \langle \rho \rangle_l P^{\alpha\beta} - \frac{\partial}{\partial x_k}\left(\langle \rho \rangle_l \tau_L\ \ u_k, \phi_\alpha, \phi_\beta\ \ - \mu \frac{\partial \tau_L\ \ \phi_\alpha, \phi_\beta}{\partial x_k} \right)$$

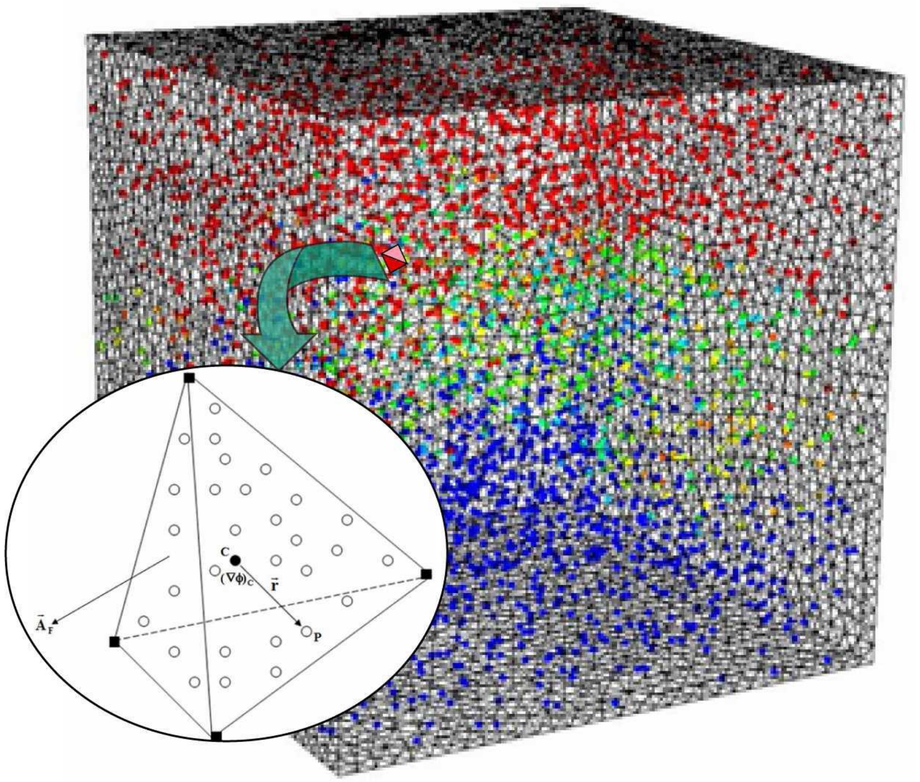
$$+ 2\mu \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_k} \frac{\partial \langle \phi_\beta \rangle_L}{\partial x_k} - 2 C_\phi \omega \langle \rho \rangle_l \tau_L\ \ \phi_\alpha, \phi_\beta$$

$$\frac{\partial \langle \rho \rangle_l \tau_L\ \ u_i, \phi_\alpha}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_k \rangle_L \tau_L\ \ u_i, \phi_\alpha}{\partial x_k} = \langle \rho \rangle_l P_i^\alpha - \frac{\partial}{\partial x_k}\left(\langle \rho \rangle_l \tau_L\ \ u_k, u_i, \phi_\alpha\ \ - \mu \frac{\partial \tau_L\ \ u_i, \phi_\alpha}{\partial x_k} \right)$$

$$+ G_{ik} \langle \rho \rangle_l \tau_L\ \ u_k, \phi_\alpha\ \ - C_\phi \omega \langle \rho \rangle_l \tau_L\ \ u_i, \phi_\alpha$$

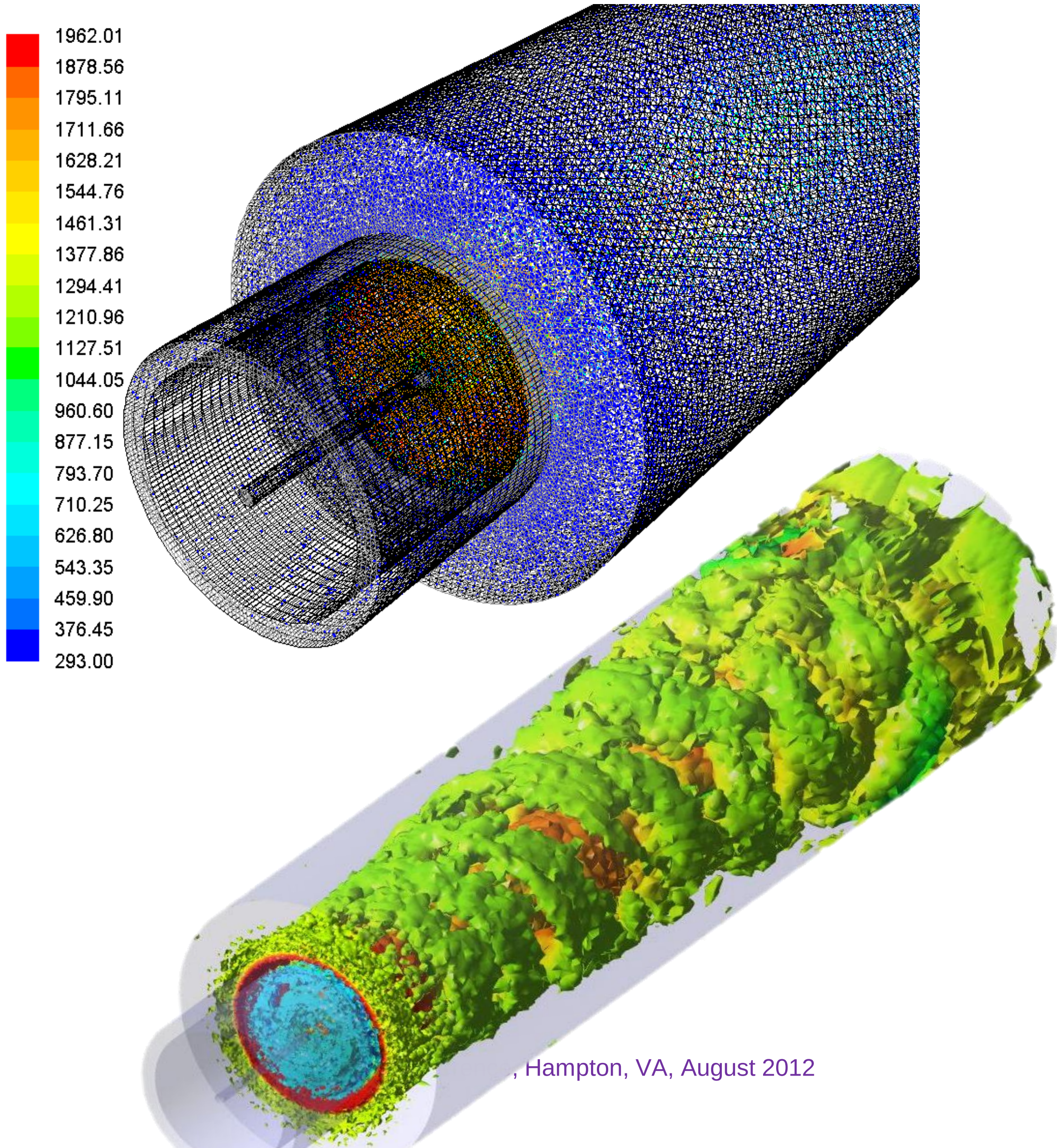
FDF Simulation

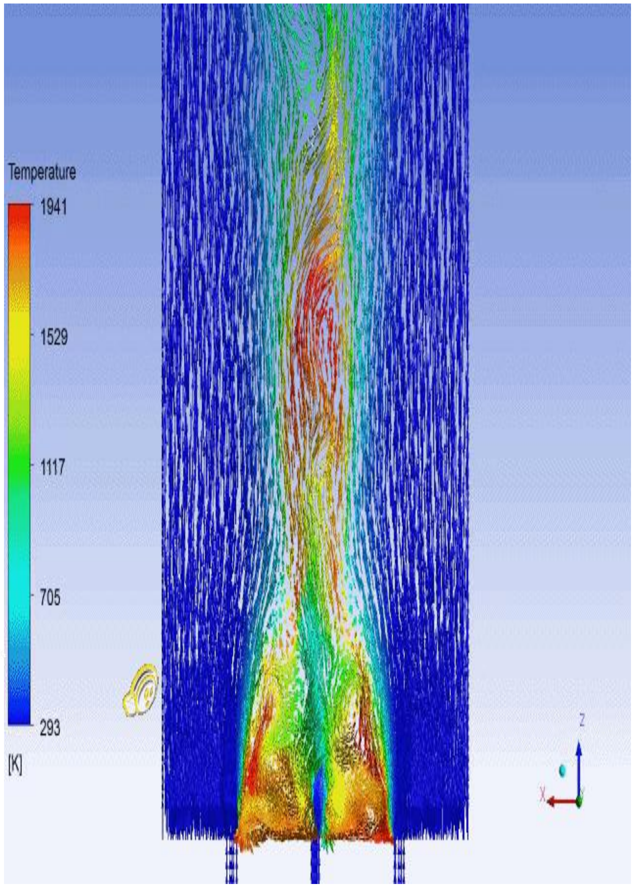
Typically Lagrangian Monte Carlo elements on Eulerian grids.



- Complex domain.
- 10**9   grids /elements.
- 10**11 MC particles.
- Mostly reduced kinetics.

Example 1: Sydney-Sandia Swirl Burner

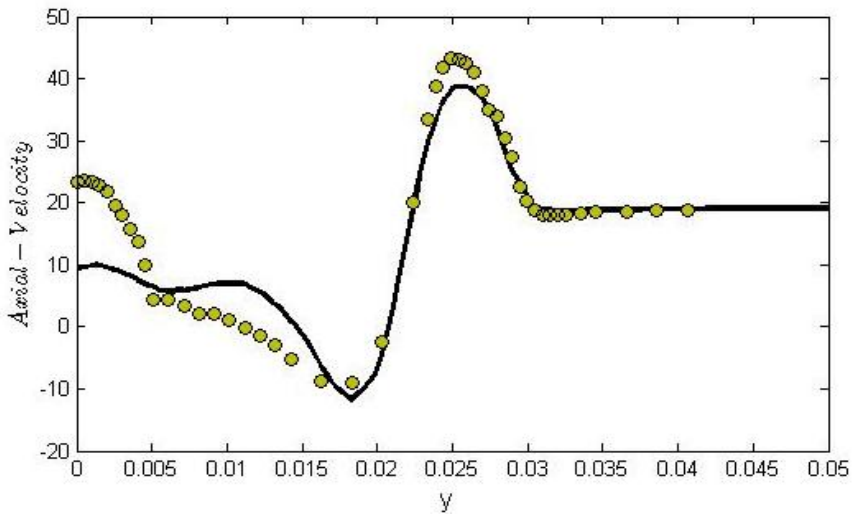


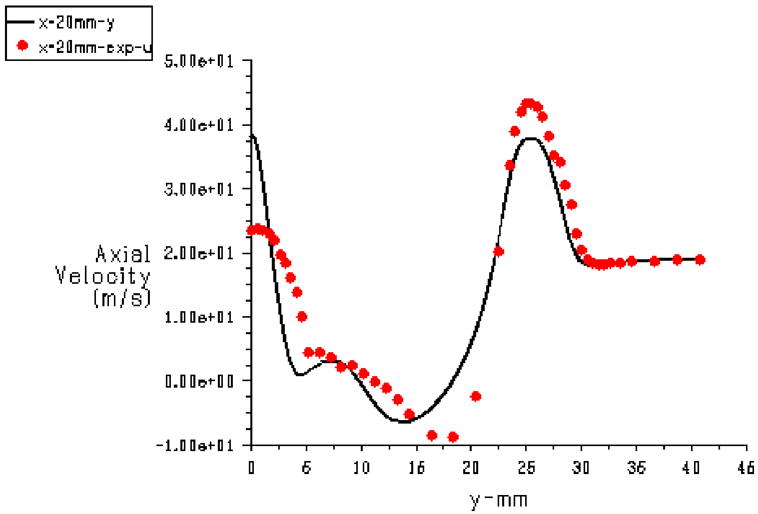


FDF vs. RANS: Axial Velocity

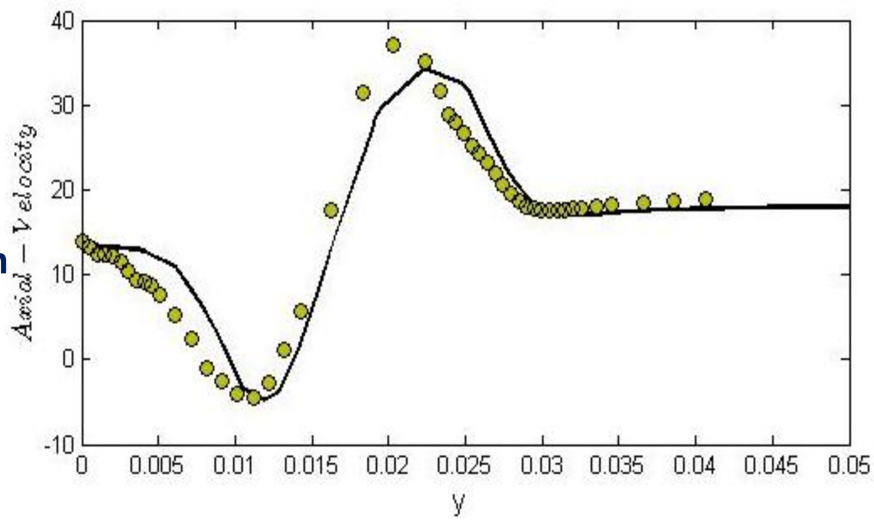
LES / FDF | **RANS**

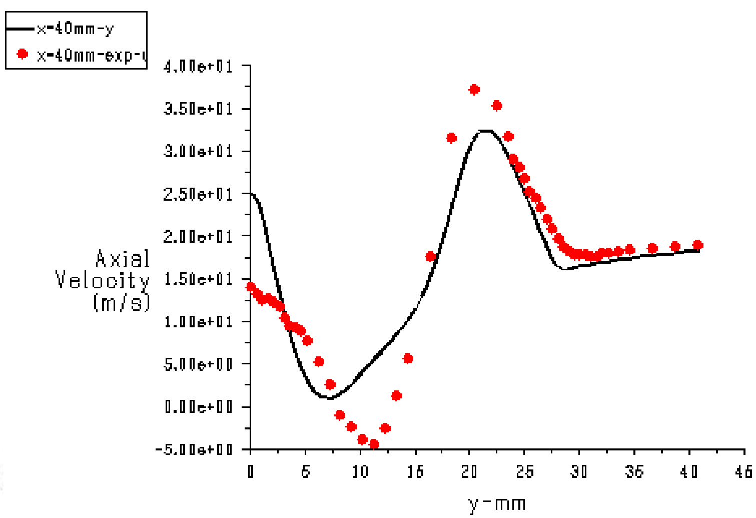
Z = 20 mm





Z = 40 mm

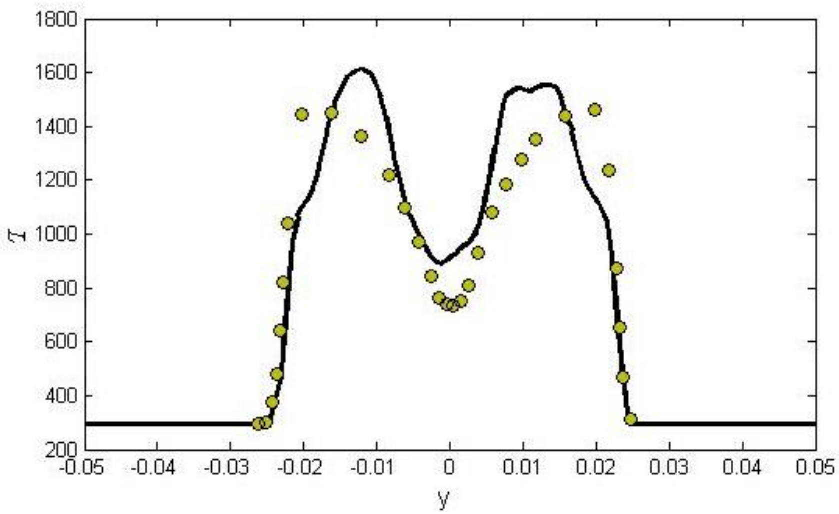


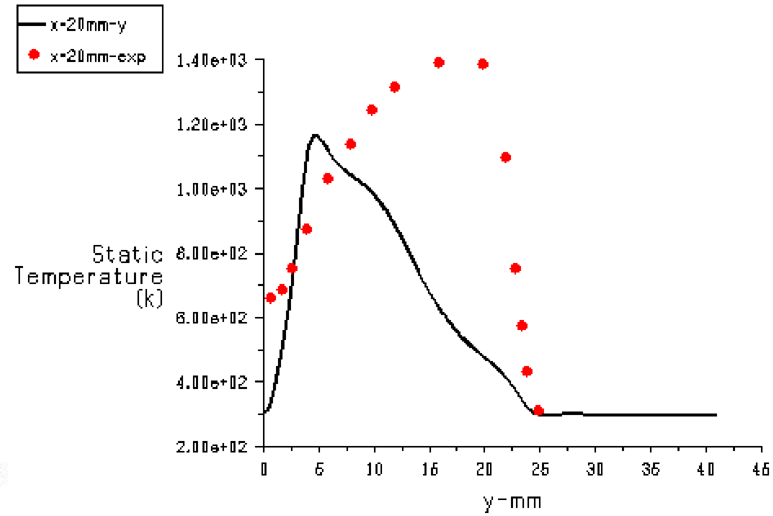


FDF vs. RANS : Temperature

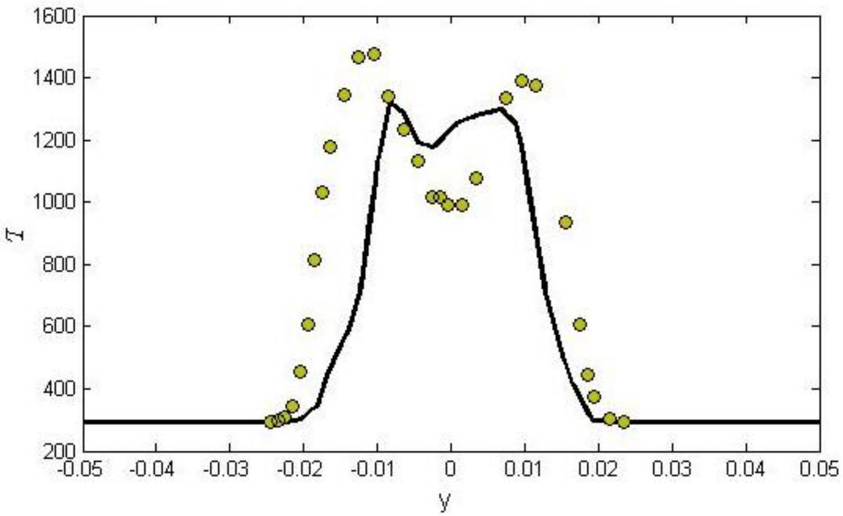
LES / FDF | **RANS**

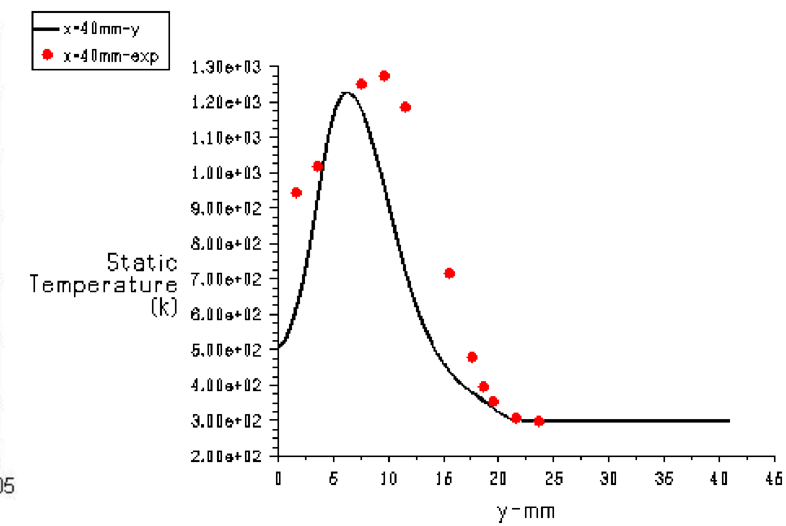
Z = 20 mm





Z = 40 mm

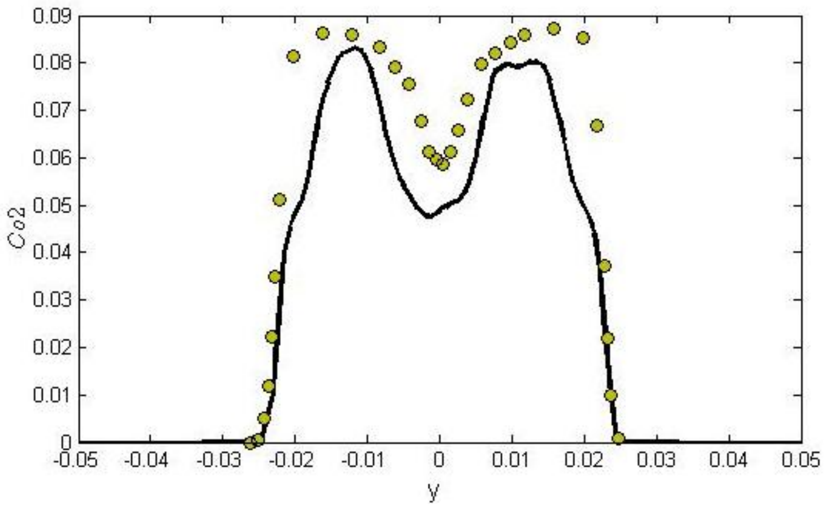


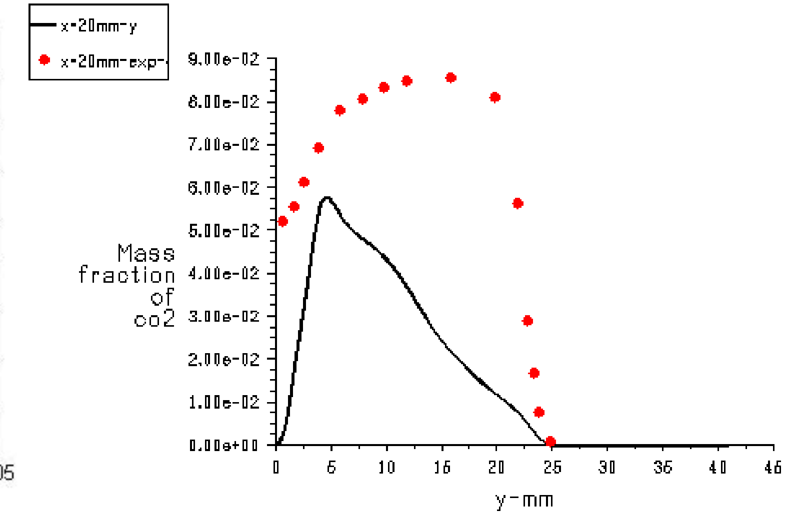


FDF vs. RANS: CO2 Mass Fraction

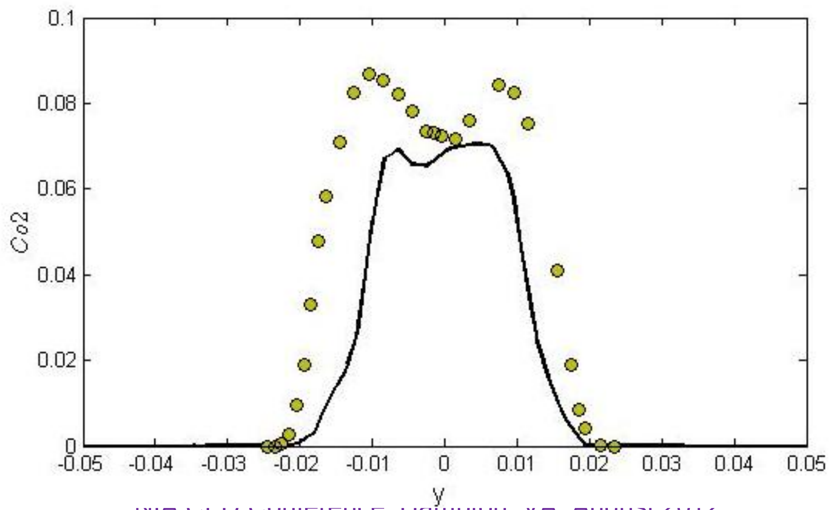
LES / FDF | **RANS**

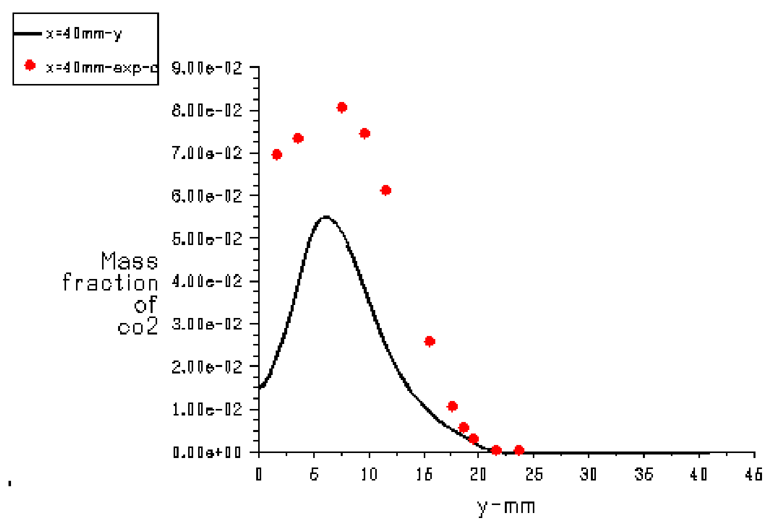
Z = 20 mm



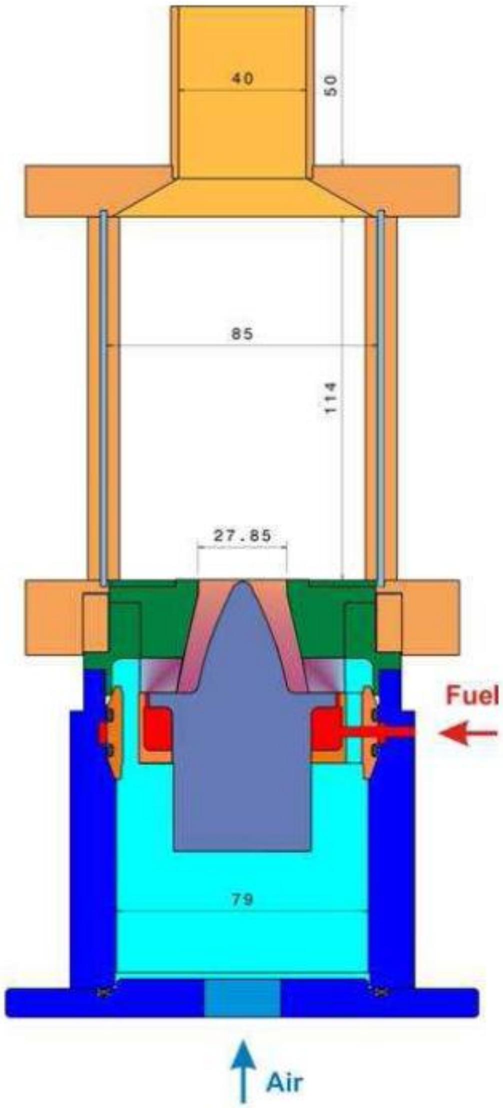


Z = 40 mm





Example 2: DLR PRECCINSTA Burner



Reasonable representation of an industrial type gas turbine combustor.

Combustor features a plenum, a swirler & a square combustion chamber.

CH_4 fuel at equivalence ratio of 0.83 fed through 12 injection holes within the radial swirler.

Dry air at ambient temperature fed via the plenum through the radial swirlers.

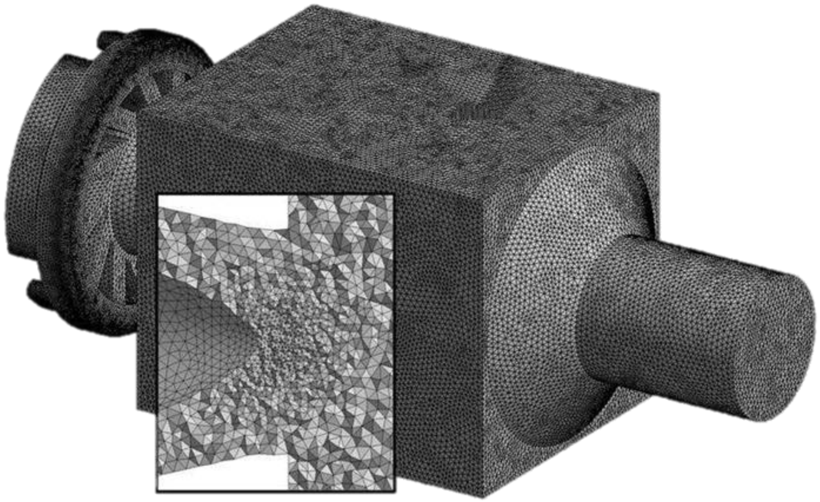
Total mass flow rate = 12.9 g/s

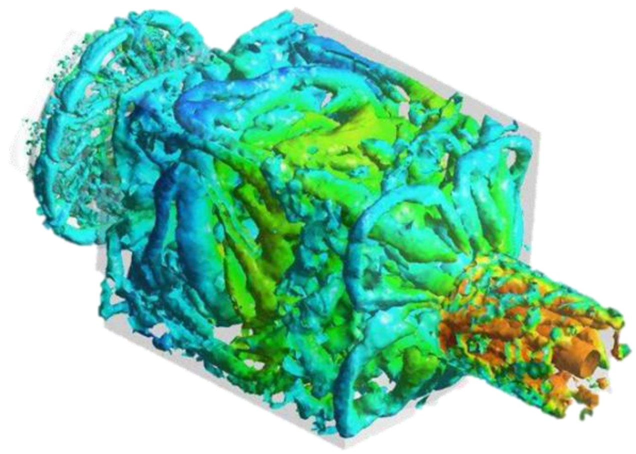
Combustion chamber cross section = 85 mm x 85 mm

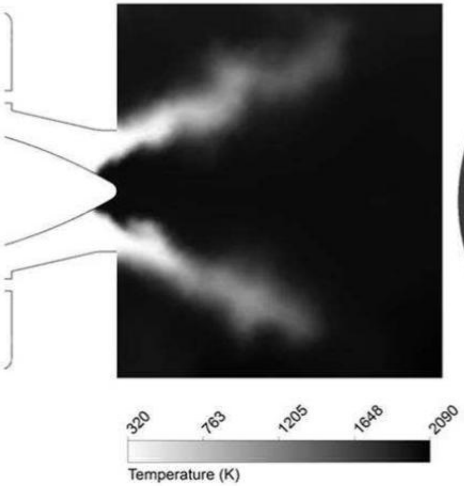
Combustion chamber height = 114 mm

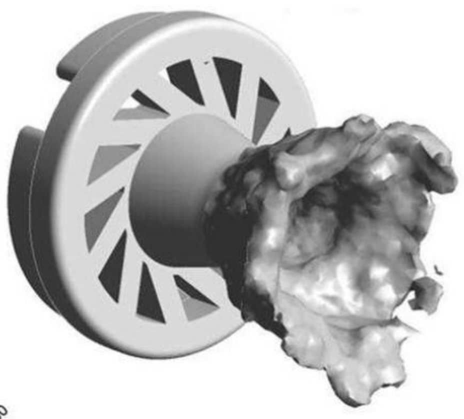
PITT

DLR Flame

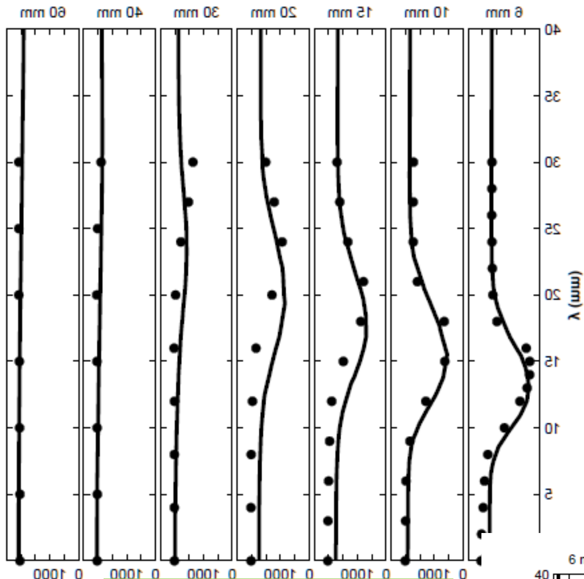




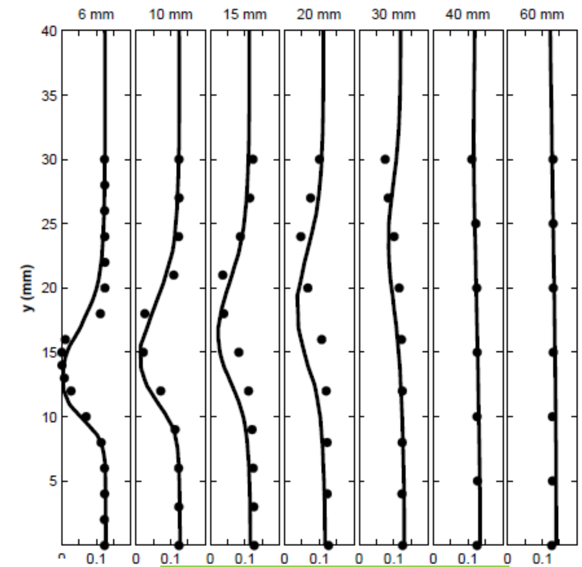




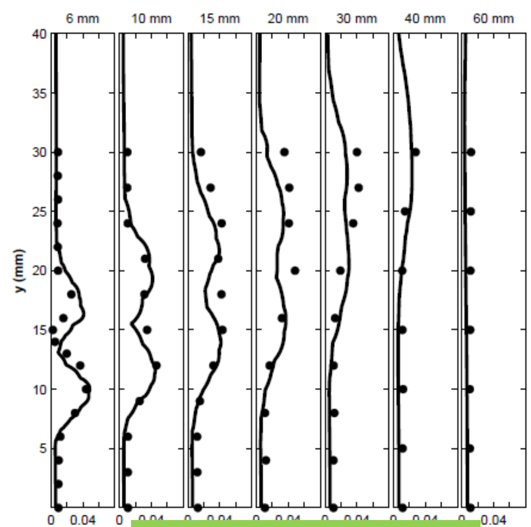
DLR Flame



MEAN Temperature

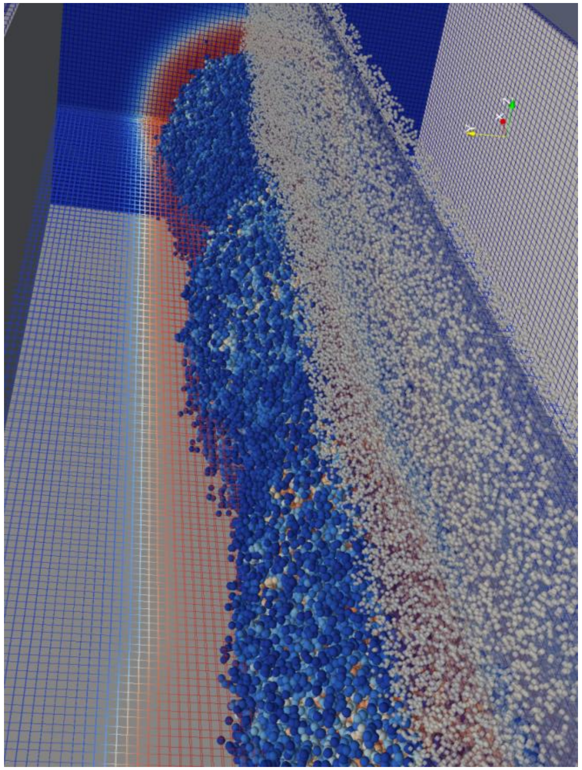


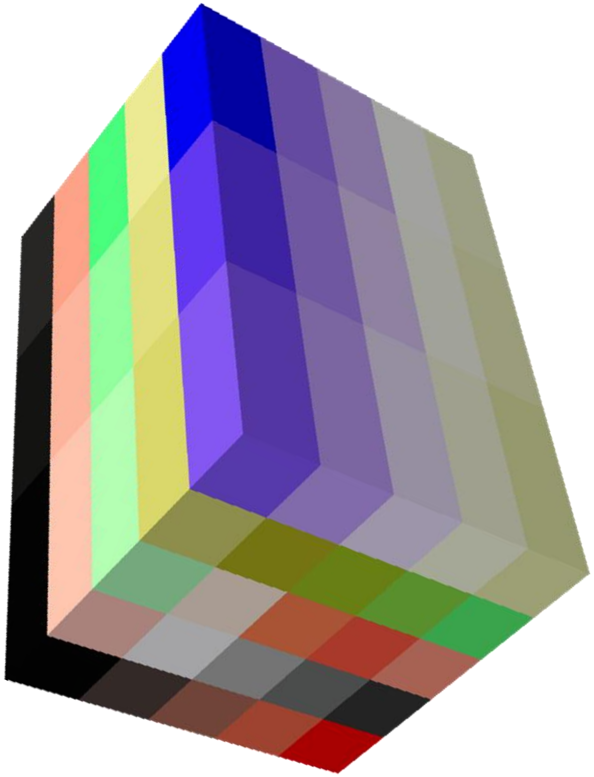
MEAN CO_2

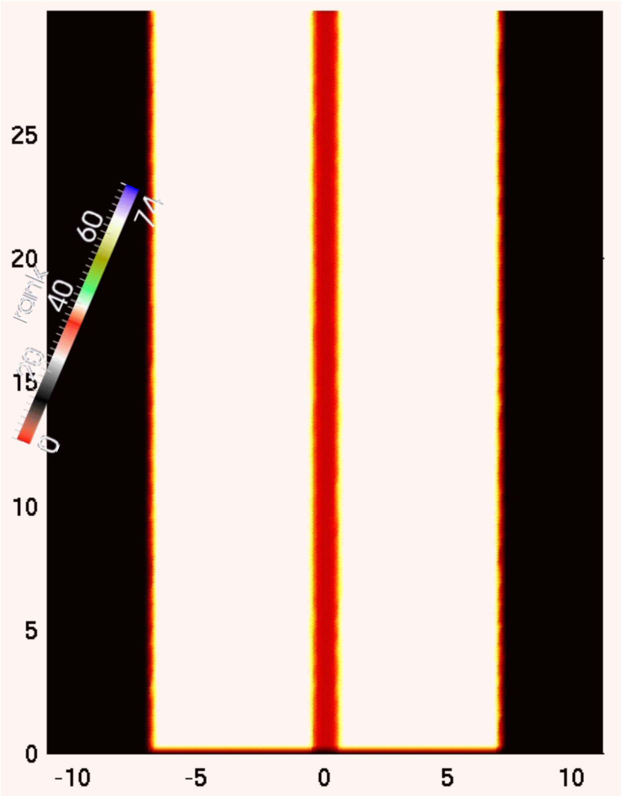


RMS CO_2

Towards Petascale FDF Simulation







Typically the domain is *regularly* portioned

Inefficient on massively parallel platform

Irregularly Portioned Processors

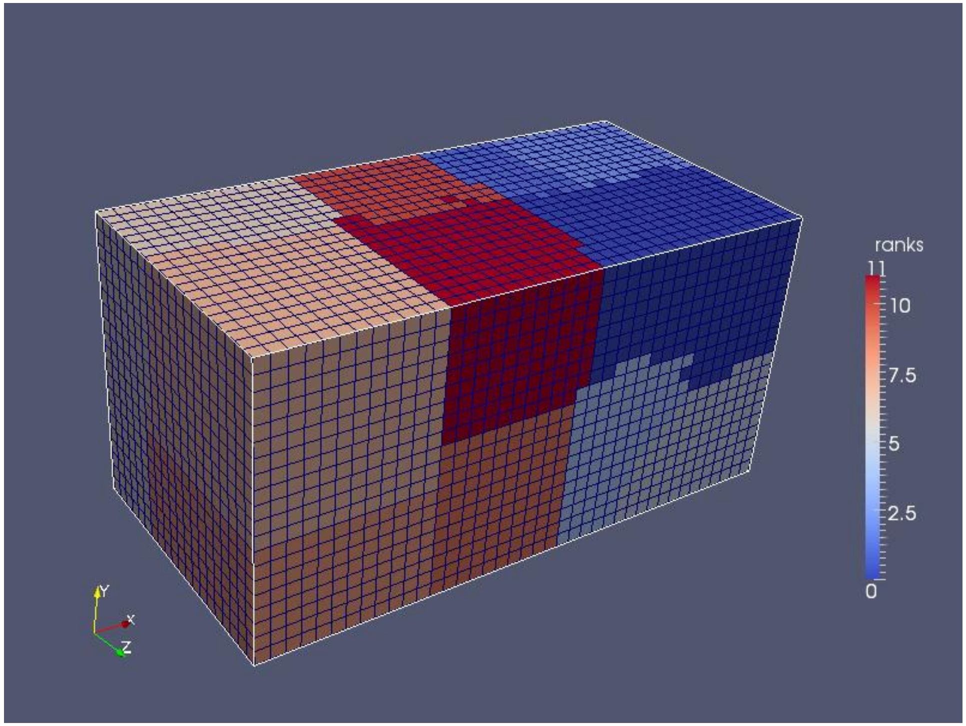
Partition in to subdomains

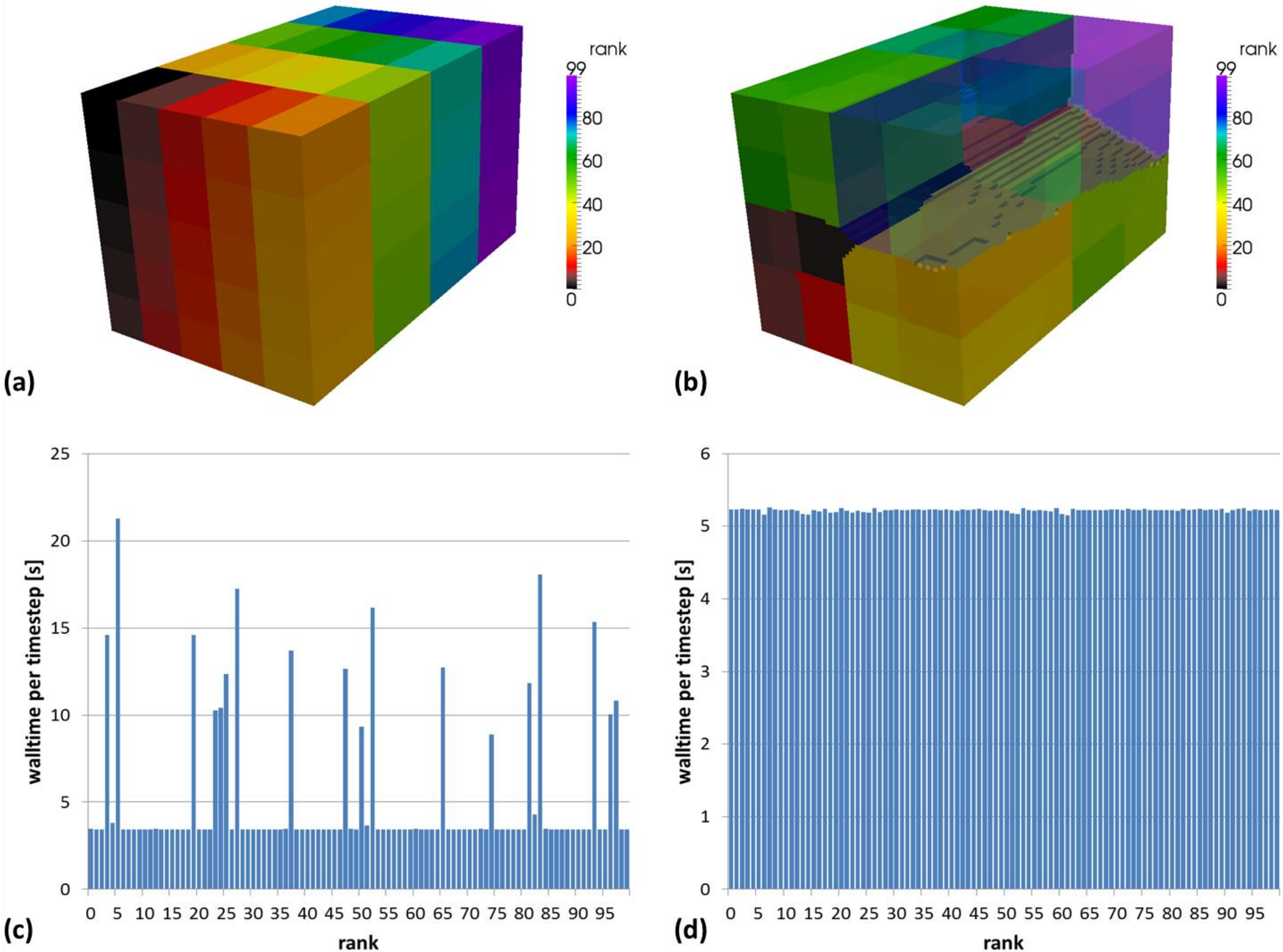
Connectivity between subdomains:

- Local data
- Neighboring data
- Communication patterns

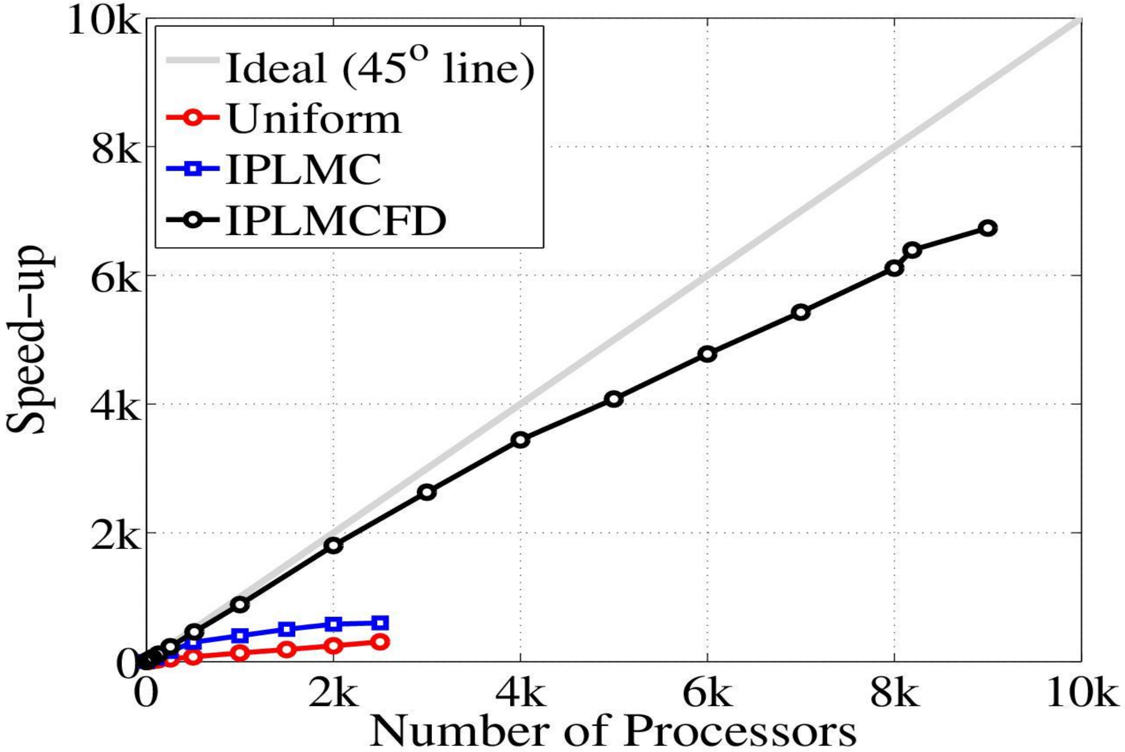
Data structures

- 1D arrays that map to a global 3D array
- Particle lists
- Array of particle lists (bins)

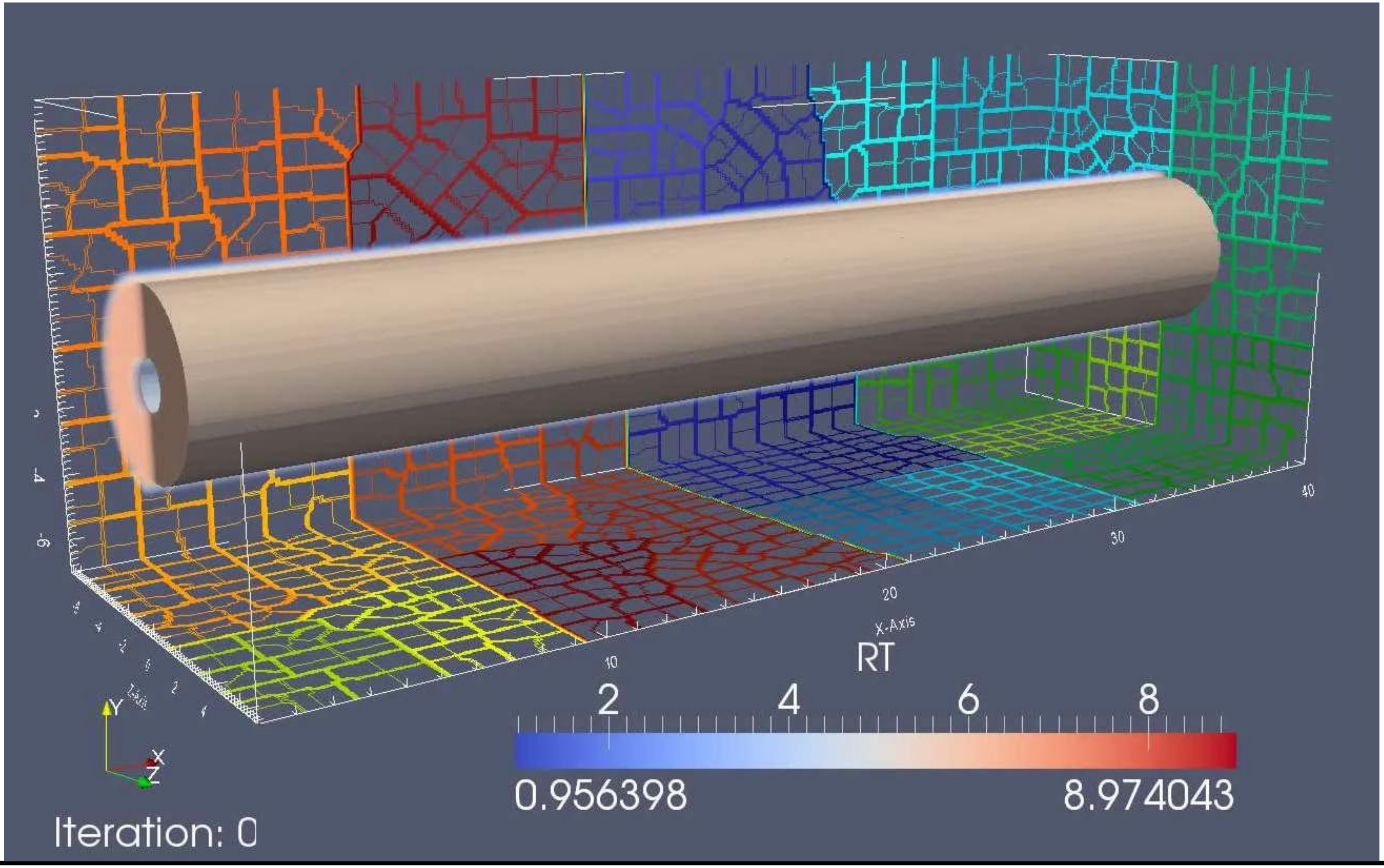



(a)
(b)
(c)
(d)
rank
99
80
60
40
20
0
walltime per timestep [s]
rank

Scalability

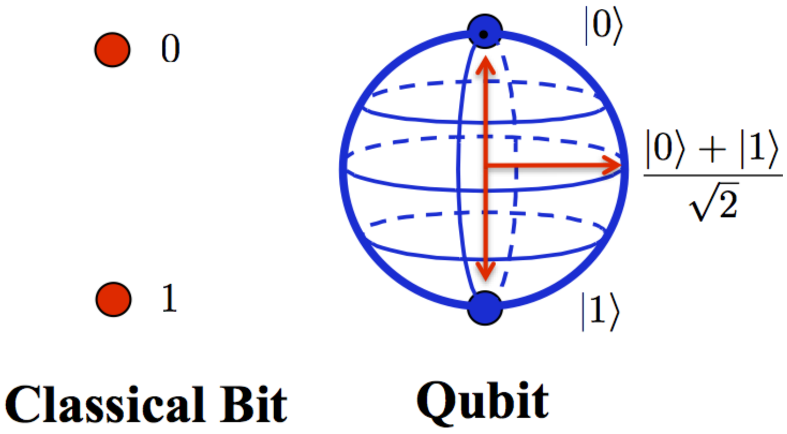


Example: Bunsen Burner



Quantum Computing

- Quantum computers use special properties of microscopic objects to process information



- Information in a classical computer is stored as bits
- In a quantum computer it is stored as qubits

A qubit can be in a superposition of 0 and 1

Example 1:

- Perform certain tasks much faster than a normal (classical) computer
- e.g., quantum computers can factor numbers *exponentially* faster than classical computers (Shor, 1994)

Difficulty of factoring numbers is foundation of public key encryption

3846852236028771306714522764917795580121348770 1099
8995628016726328849290641325010623473892362548 7248

38468522360287713067145227649177955801213487701099
89956280167263288492906413250106234738923625487248
43632748829239471099553846946567828308577705718806
94978568779355941701709253073909647758709792262685
32784959698795712324287283270444145525795129254121
12071034603788102611457488328357687802285073243 1110
88058576663938238037682029535630748718401810408271
76190278143998393196563941173000272355947393 84321

=

19151078601511813582801009133095143365412697691872
82849826678249401200032709416910316550320010920704
37797665474841228343134658535223112172218027305038
34496265576199132087913176183816562977572021862399

X

20086869862907331390554301660726422765403303838159
28513728233298852507348154165945582548188931037072
13279188964772171854249281063180682234029182739436
25886101798462506273138523315831932882407840022527
9

Example 2:

DATABASE SEARCH
(Grover)
Telephone book
with *N*=1,000,000 entries

***Task*: find name of person whose number is: (757) 864-6228**

Ordinary Phonebook

Number found after
~N/2=500,000 attempts

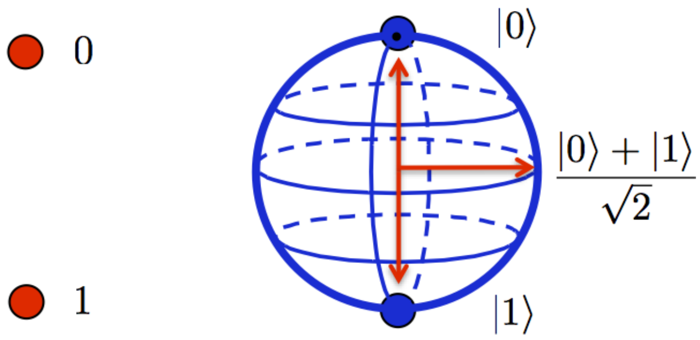
Quantum Phonebook

Number found after
~$N^{1/2}$ =1000 attempts

- *Other algorithms with quantum speed-ups for: sparse linear equations, classical simulated annealing, quantum Monte-Carlo computations,…*

Power of Quantum Computers

- They can represent many outcomes at once



Classical Bit **Qubit**

- Single qubit: 2D space

$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle$$

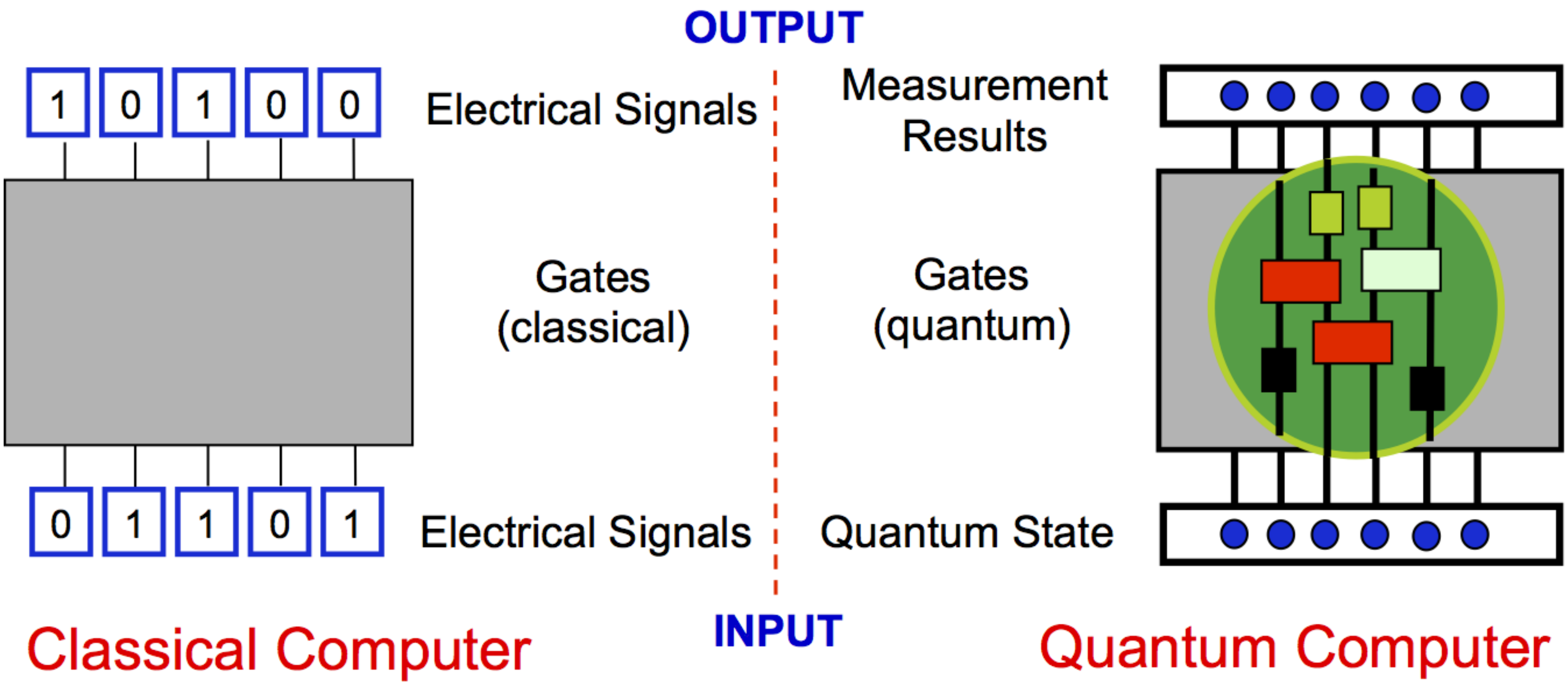
$$|a_0|^2 + |a_1|^2 = 1$$

- Many qubits: 2^n complex numbers describe the state

$$|\psi\rangle = a_0|000\ldots000\rangle + a_1|000\ldots001\rangle + a_2|000\ldots010\rangle + \ldots + a_{2^n-1}|111\ldots111\rangle$$

A state with n=1000 qubits is specified by $2^{1000} \sim 10^{300}$ coefficients !

Operation


OUTPUT
1 0 1 0 0
Electrical Signals
Measurement Results
Gates (classical)
Gates (quantum)
0 1 1 0 1
Electrical Signals
Quantum State
INPUT
Classical Computer
Quantum Computer

General Structure: Classical

Step 1: Initialize (boot) computer.

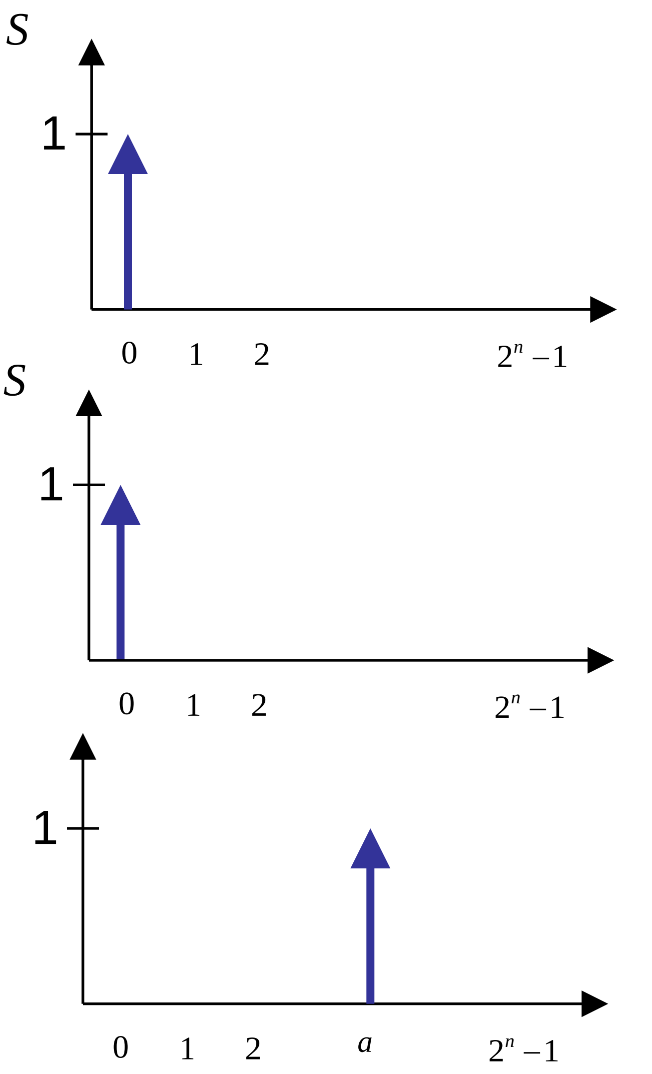
$$S(0) = 1$$

Step 2: Gate operations

$$S \to F \;\; S$$

Step 3: Read out answer a

$$F \;\; S \;\; (a) = 1$$



General Structure: Quantum

Step 1: Initialize quantum computer.

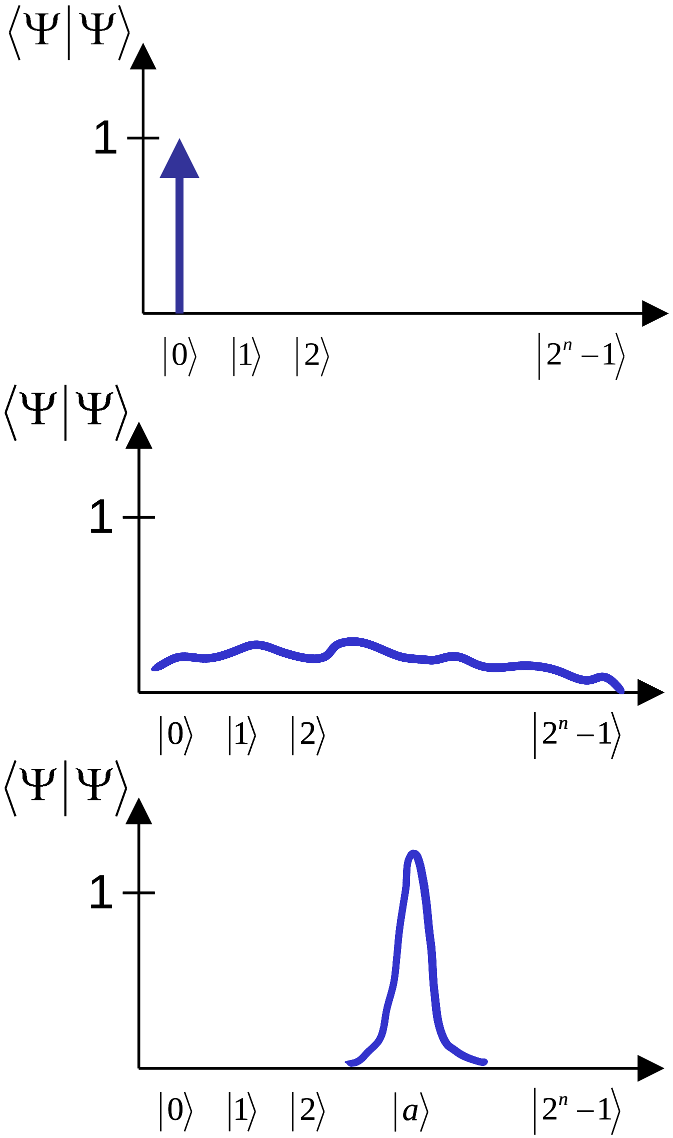
$$|\Psi_0\rangle = |0\rangle$$

Step 2: Quantum gate operations

$$i\hbar \frac{\partial|\Psi\rangle}{\partial t} = \hat{H}\ t\ |\Psi\rangle$$

Step 3: Quantum measurement

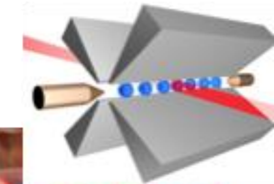
$$P\ a\ = |\langle a|\Psi\rangle|^2$$

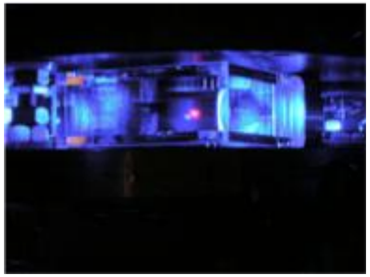


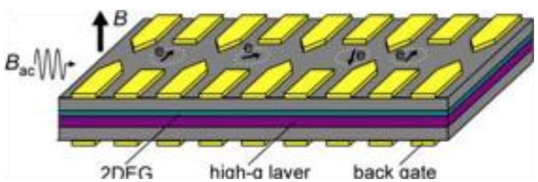
Hardware

Many implementations are being explored, with components already demonstrated:

- Neutral atoms
- Trapped ions
- Color centers (e.g., NV-centers in diamond)
- Quantum dots
- Superconducting qubits (charge, phase, flux)
- Nuclear Magnetic Resonance systems
- Optical qubits

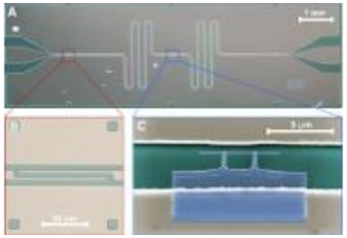


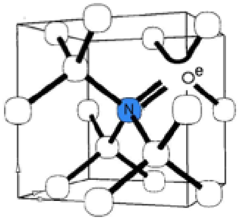


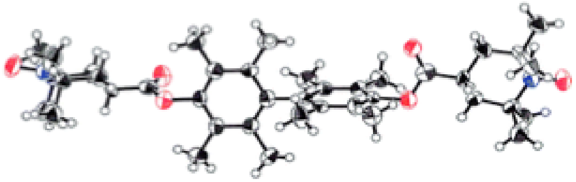


State of the art

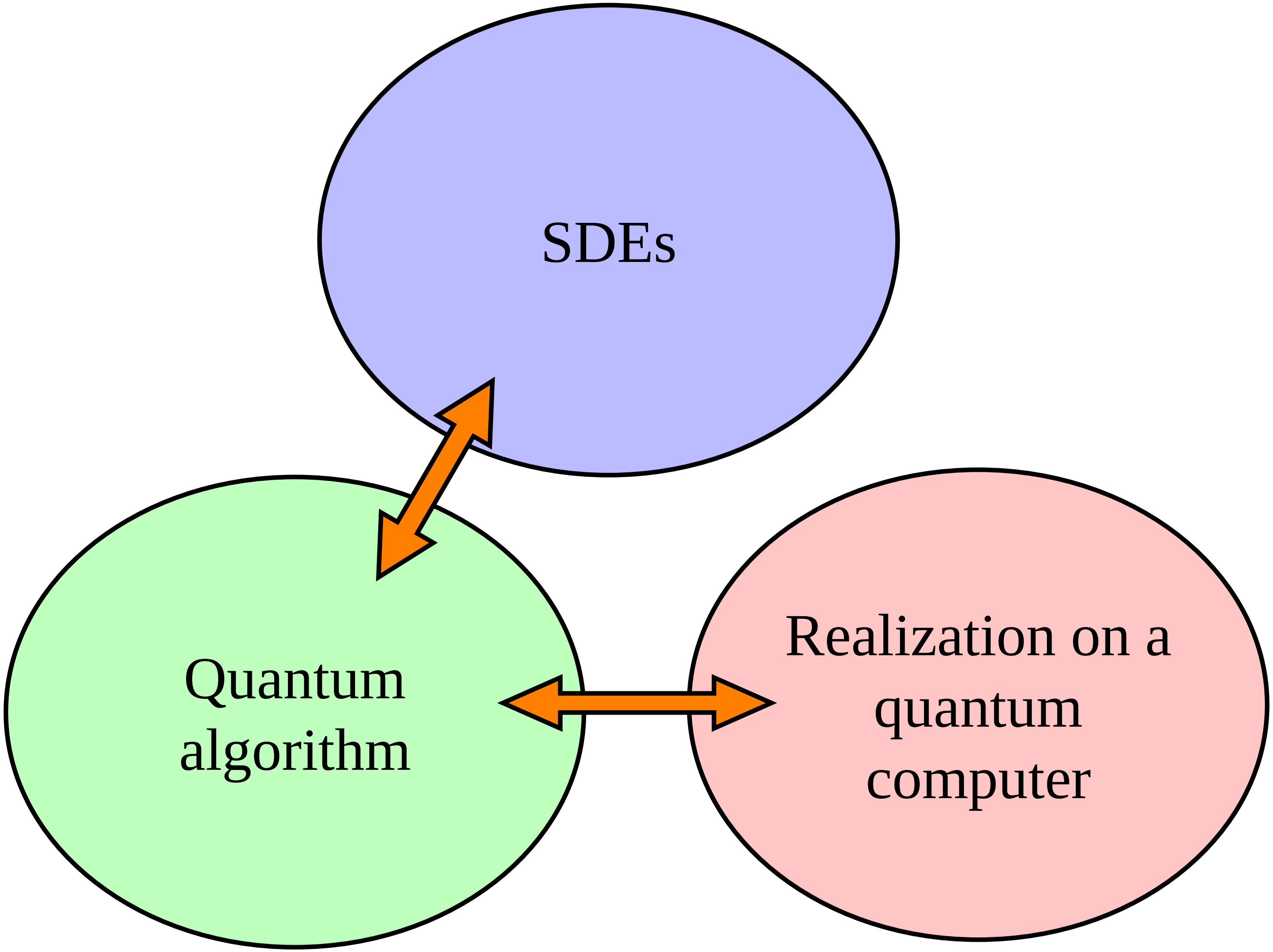
- 14 entangled qubits with several hundred gate operations – trapped ions
- Large qubit arrays (ca. 500) with neutral atoms (but slow gate timescales)
- Fast gate operations demonstrated with superconducting qubits







Quantum Speedup for FDF?



Summary of FDF Properties

- Turbulence-Chemistry interactions in closed form.
- SGS scalar fluxes in closed form.
- Equivalent to 2^{nd} order closures (at least).
- Quantum computing may be very effective for FDF simulation.
- Applicable to premixed, non-premixed, and partially premixed flames.
- Applicable to both flamelet and distributed flame regions.
- Continues to gain popularity in turbulence simulation.

Popularity of FDF

- UC Berkeley
- Stanford
- Purdue
- Iowa State
- Cornell
- UT Austin
- SUNY-Buffalo
- U. Wyoming
- Michigan State
- CTR/NASA Ames
- NASA Langley
- Sandia Labs
- Rolls Royce
- ANSYS
- .
- .
- .

- England
- France
- Germany
- Netherland
- Portugal
- Russia
- Spain
- Kazakhstan
- Canada
- China
- .
- .
-
- in FLUENT
- In US3D
- In VULCAN .