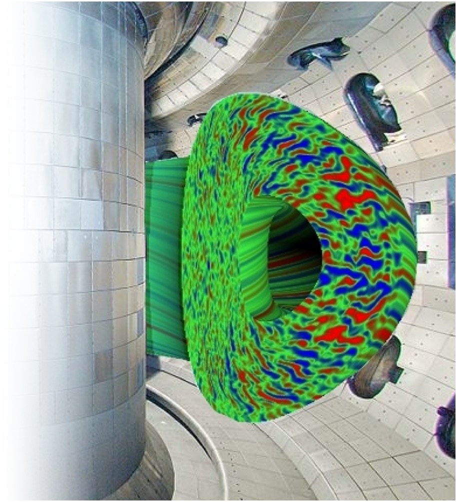
Advancing Fusion Science with CGYRO using GPU-Based Leadership Systems



by
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- Chris Holland (UCSD)
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- Walter Guttenfelder, Brian Grierson (PPPL)
- George Fann (ORNL)
- Klaus Hallatschek (IPP, Germany)

OUTLINE

1. Who is General Atomics?

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2. The case for **fusion energy**

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3. Mathematical formulation and GPU-based numerical solution

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4. Simulation of turbulent energy loss in a tokamak plasma
5. GPU performance: development and results

Who is General Atomics?

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2. The GA **Magnetic Fusion** division does DOE-funded research
3. Hosts **DIII-D National Fusion Facility**

Founded on July 18, 1955 (photo 1957)

The General Atomic Division of General Dynamics

Laboratory formally dedicated on June 25th, 1959

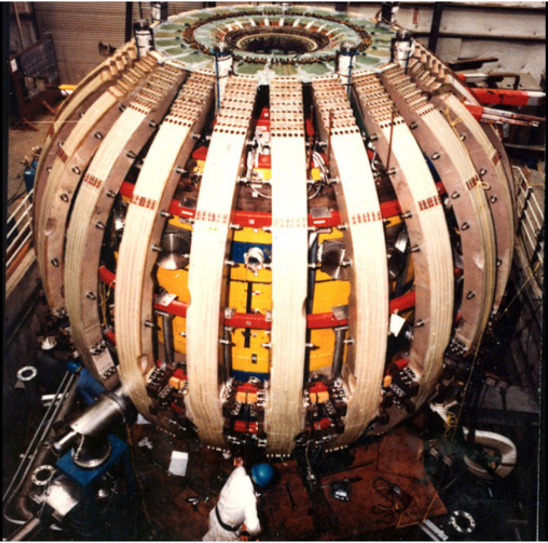
John Jay Hopkins Laboratory for Pure and Applied Science

Present-day Campus (2019)

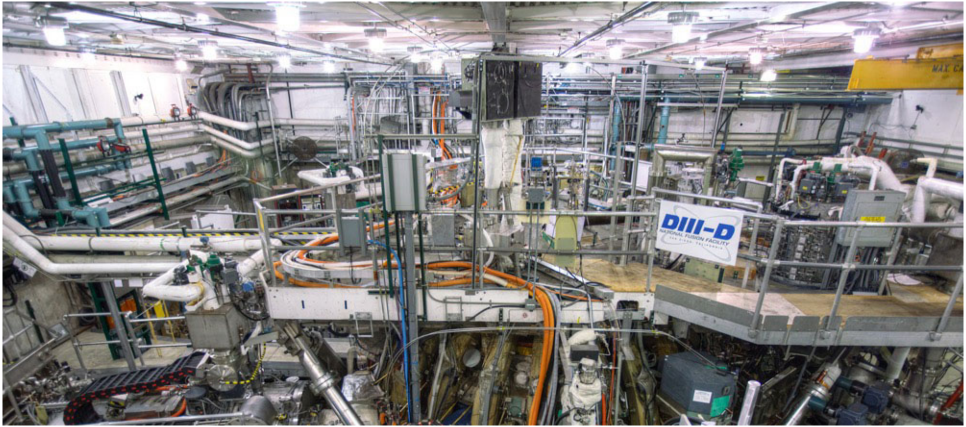
Retains feel of early architecture

GENERAL ATOMICS

Doublet III (1974)



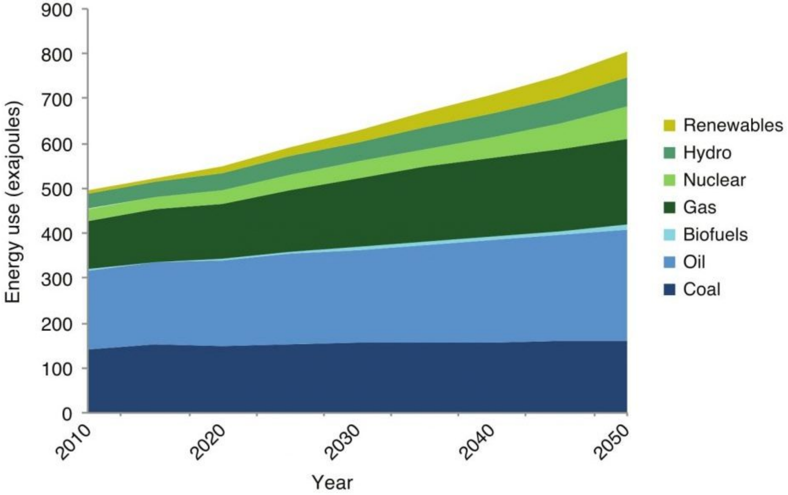
DIII-D (Present day)



The case for fusion energy

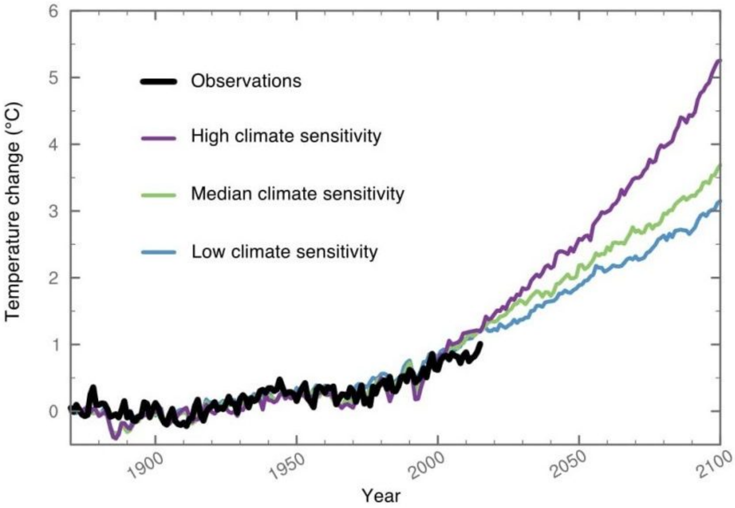
Energy Use by Technology and Year

energy.mit.edu/news/limiting-global-warming-aggressive-measures-needed

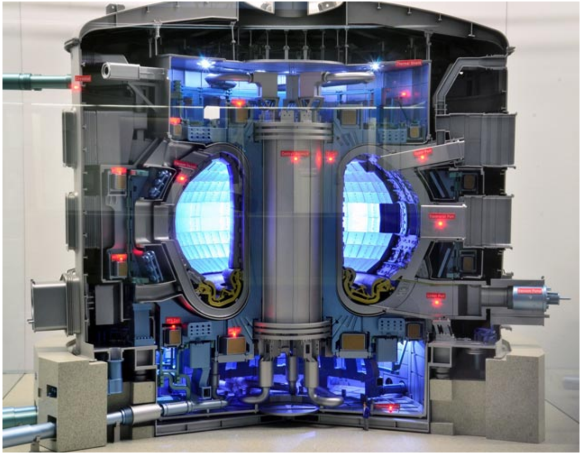


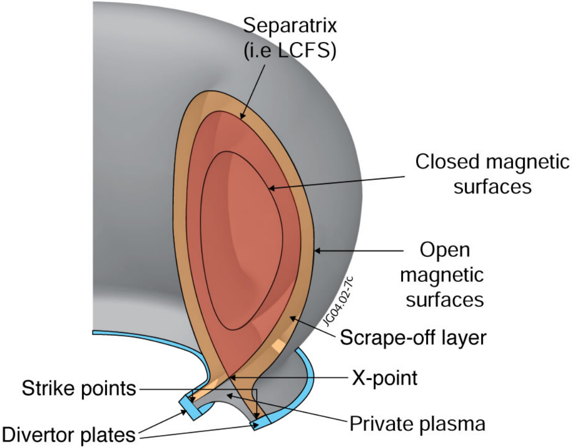
Surface Temperature Anomaly

energy.mit.edu/news/limiting-global-warming-aggressive-measures-needed

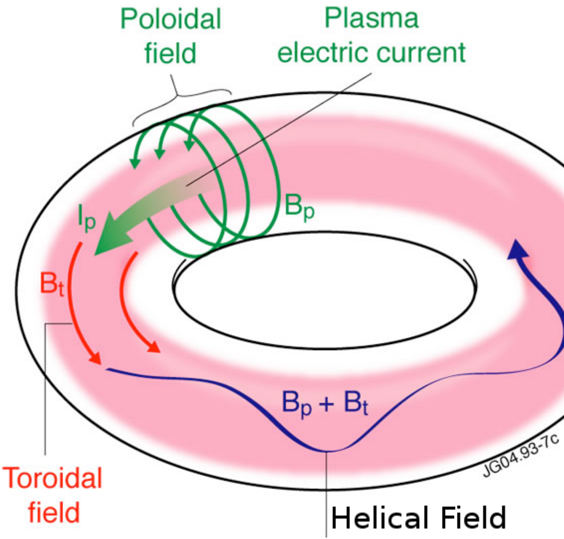


Plasma theory in closed fieldline region well-understood

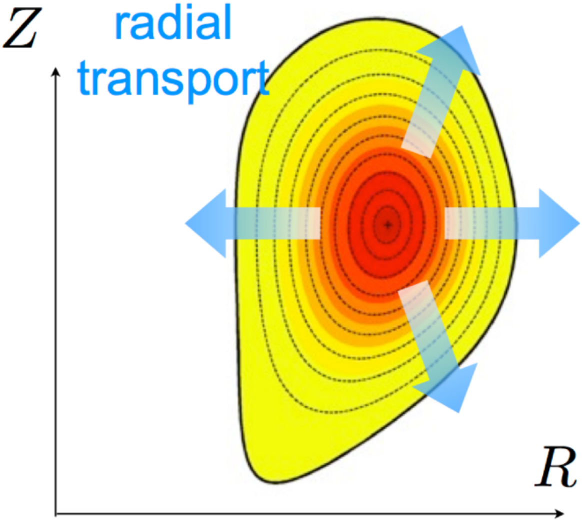




Helical field perfectly confines plasma (almost)



There is a small amount of radial energy/particle loss



- Collisions (1970s): $\Gamma_{\text{collision}}$
- Turbulence (1980s): $\Gamma_{\text{turbulence}}$
- Both exhibit **gyroBohm scaling**

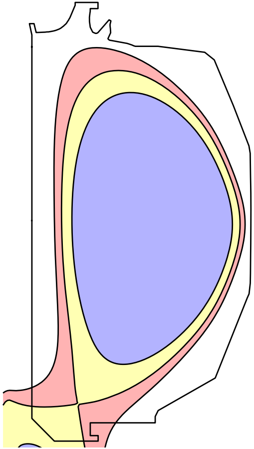
flux $\Gamma \sim v(\rho/a)^2$

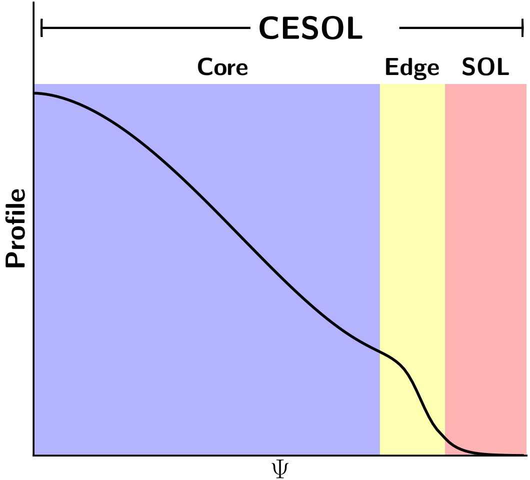
confinement time $\tau = \frac{a}{\Gamma} \sim \frac{a^3}{v\rho^2}$

- a = torus radius
- ρ = particle orbit size
- v = particle velocity

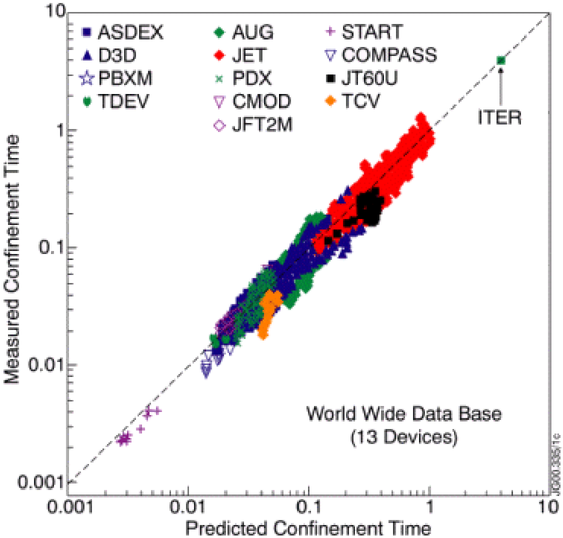
Tokamak physics spans multiple space/timescales

Core-edge-SOL (CESOL) region coupling





Tokamak confinement improves with LARGE PLASMA VOLUME



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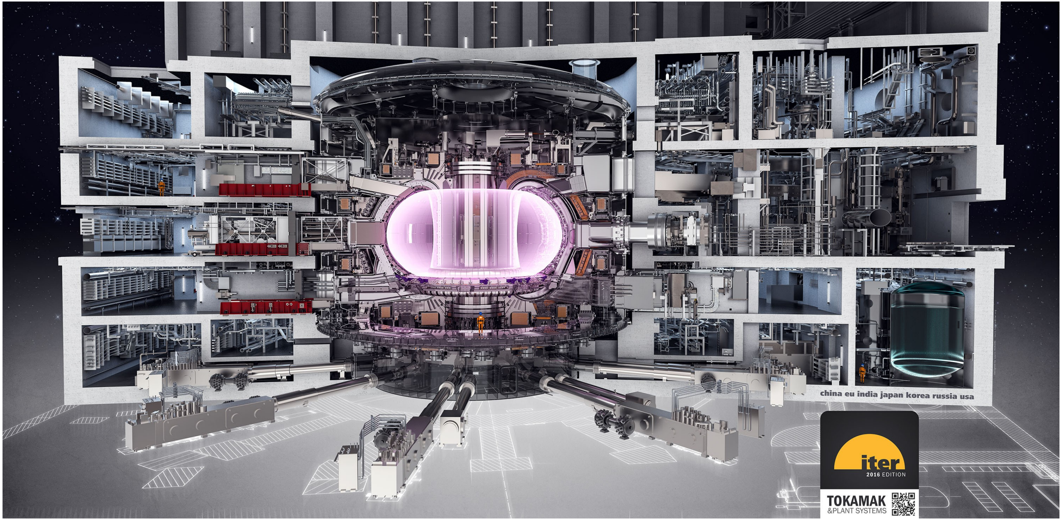
ITER Facility (35 nations) under construction in France

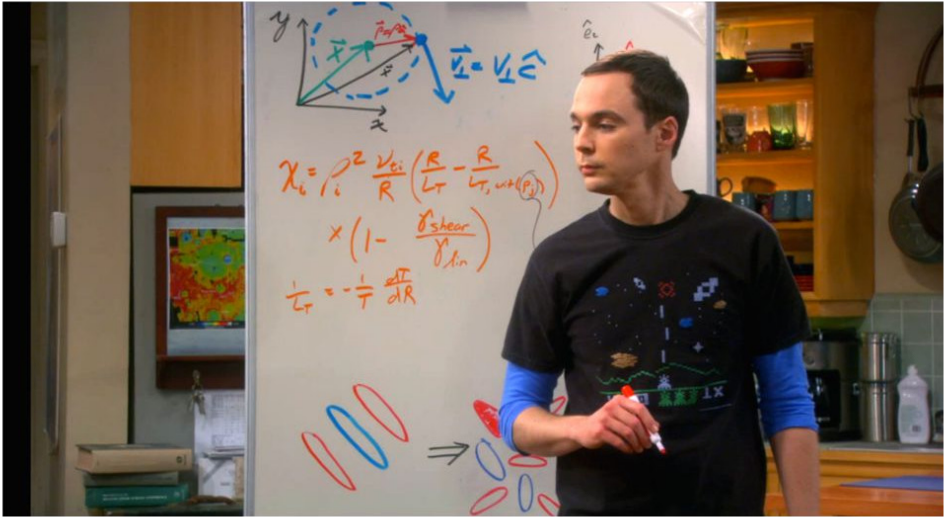
GOAL: Simulate turbulent plasma in core (magenta) region



Mathematical formulation and GPU-based numerical solution

Gyrokinetic Theory for Magnetized Plasma

The Cooper/Kripke Inversion



Gyrokinetic equation for plasma species a

Typically: $a = (\text{deuterium, carbon, electron})$

$$\frac{\partial \widetilde{h}_a}{\partial \tau} - i\Omega_s X \widetilde{h}_a - i\left(\Omega_\theta + \Omega_\xi + \Omega_d\right) \widetilde{H}_a - i\Omega_* \widetilde{\Psi}_a + \Omega_{NL}\left(\widetilde{h}_a, \widetilde{\Psi}_a\right) = \mathcal{C}_a$$

Symbol definitions

particles $$\widetilde{H}_a = \widetilde{h}_a + \frac{z_a T_e}{T_a}\widetilde{\Psi}_a$$

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Symbol definitions

particles $$\widetilde{H}_a = \widetilde{h}_a + \frac{z_a T_e}{T_a}\widetilde{\Psi}_a$$

fields $$\widetilde{\Psi}_a = J_0(\gamma_a)\left(\delta\widetilde{\phi} - \frac{v_\parallel}{c}\delta\widetilde{A}_\parallel\right) + \frac{v_\perp^2}{\Omega_{ca} c}\frac{J_1(\gamma_a)}{\gamma_a}\delta\widetilde{B}_\parallel$$

Electromagnetic GK-Maxwell Equations

Coupling to fields is a MAJOR complication!

$$\left(k_\perp^2\lambda_D^2 + \sum_a z_a^2 \frac{T_e}{T_a}\int d^3v \frac{f_{0a}}{n_e}\right) \delta\widetilde{\phi} = \sum_a z_a \int d^3v \frac{f_{0a}}{n_e} J_0(\gamma_a)\, \widetilde{H}_a$$

$$\frac{2}{\beta_{e,\mathrm{unit}}} k_\perp^2 \rho_s^2 \, \delta\widetilde{A}_\| = \sum_a z_a \int d^3v \frac{f_{0a}}{n_e} \frac{v_\|}{c_s} J_0(\gamma_a)\, \widetilde{H}_a$$

$$-\frac{2}{\beta_{e,\mathrm{unit}}} \frac{B}{B_\mathrm{unit}} \, \delta\widetilde{B}_\| = \sum_a \int d^3v \frac{f_{0a}}{n_e} \frac{m_a \mathrm{v}_\perp^2}{T_e} \frac{J_1(\gamma_a)}{\gamma_a}\, \widetilde{H}_a$$

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Typically, deuterium, some carbon, and electrons

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E × B flow

$$-i\Omega_s = -i\,\frac{k_\theta L}{2\pi}\frac{a}{c_s}\gamma_E$$

Gyrokinetic equation for plasma species a

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$$\frac{\partial \widetilde{h}_a}{\partial \tau} - i\Omega_s X \widetilde{h}_a - i\left(\Omega_\theta + \Omega_\xi + \Omega_\mathrm{d}\right)\widetilde{H}_a - i\Omega_*\widetilde{\Psi}_a + \Omega_\mathrm{NL}(\widetilde{h}_a, \widetilde{\Psi}_a) = \mathcal{C}_a$$

Streaming

$$-i\Omega_\theta = \frac{v_\parallel}{w_s}\frac{\partial}{\partial\theta}$$

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$$\frac{\partial \widetilde{h}_a}{\partial \tau} - i\Omega_s X \widetilde{h}_a - i\left(\Omega_\theta + \Omega_\xi + \Omega_\mathrm{d}\right)\widetilde{H}_a - i\Omega_* \widetilde{\Psi}_a + \Omega_\mathrm{NL}(\widetilde{h}_a, \widetilde{\Psi}_a) = \mathcal{C}_a$$

Trapping

$$-i\Omega_\xi = -\frac{v_{ta}}{\mathrm{w}_s}\frac{u_a}{\sqrt{2}}\left(1-\xi^2\right)\frac{\partial \ln B}{\partial \theta}\frac{\partial}{\partial \xi} - \frac{1}{2u_a}\frac{\partial \lambda_a}{\partial \theta}\left[\frac{v_\parallel}{\mathrm{w}_s}\frac{\partial}{\partial u_a} + \frac{\sqrt{2}v_{ta}}{\mathrm{w}_s}\left(1-\xi^2\right)\frac{\partial}{\partial \xi}\right]$$

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Typically, deuterium, some carbon, and electrons

$$\frac{\partial \widetilde{h}_a}{\partial \tau} - i\Omega_s X \widetilde{h}_a - i\left(\Omega_\theta + \Omega_\xi + \Omega_\mathrm{d}\right)\widetilde{H}_a - i\Omega_* \widetilde{\Psi}_a + \Omega_\mathrm{NL}(\widetilde{h}_a, \widetilde{\Psi}_a) = \mathcal{C}_a$$

Drift motion

$$-i\Omega_\mathrm{d} = a\frac{v_{ta}}{c_s}\mathbf{b}\times\left[u_a^2\left(1+\xi^2\right)\frac{\nabla B}{B} + u_a^2\xi^2\frac{8\pi}{B^2}\left(\nabla p\right)_\mathrm{eff}\right]\cdot i\mathbf{k}_\perp\rho_a$$
$$+ M_a\frac{2av_\parallel}{c_s R_0}\mathbf{b}\times\left(\frac{R}{\mathcal{J}_\psi B}\frac{\partial R}{\partial\theta}\nabla\varphi - \frac{B_t}{B}\nabla R\right)\cdot i\mathbf{k}_\perp\rho_a$$
$$+ \frac{a}{c_s}\mathbf{b}\times\left(-\frac{v_{ta}}{T_a}\mathbf{F}_c + \frac{c}{B}\nabla\Phi_*\right)\cdot i\mathbf{k}_\perp\rho_a$$

Gyrokinetic equation for plasma species a

Typically, deuterium, some carbon, and electrons

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Gradient drive

$$-i\Omega_* = \left[\frac{a}{L_{na}} + \frac{a}{L_{Ta}}\left(u_a^2 - \frac{3}{2}\right) + \gamma_p v_\parallel \frac{a}{v_{ta}^2}\frac{RB_t}{R_0 B}\right] ik_\theta \rho_s$$
$$+ \left\{ \frac{a}{L_{Ta}}\left[\frac{z_a e}{T_a}\Phi_* - \frac{M_a^2}{2R_0^2}\left(R^2 - R(\theta_0)^2\right)\right]\right.$$
$$\left. + M_a^2 \frac{aR(\theta_0)}{R_0^2}\frac{dR(\theta_0)}{dr} + M_a \gamma_p \frac{a}{v_{ta} R_0^2}\left(R^2 - R(\theta_0)^2\right)\right\} ik_\theta \rho_s$$

Gyrokinetic equation for plasma species a

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Nonlinearity

$$\Omega_\mathrm{NL}(\widetilde{h}_a, \widetilde{\Psi}_a) = \frac{a c_s}{\Omega_{cD}} \sum_{\mathbf{k}'_\perp + \mathbf{k}''_\perp = \mathbf{k}_\perp} \left(\mathbf{b} \cdot \mathbf{k}'_\perp \times \mathbf{k}''_\perp\right) \widetilde{\Psi}_a(\mathbf{k}'_\perp) \widetilde{h}_a(\mathbf{k}''_\perp)$$

Gyrokinetic equation for plasma species a

Typically, deuterium, some carbon, and electrons

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Cross-species collision operator

$$\mathcal{C}_a = \sum_b C_{ab}^L\left(\widetilde{H}_a, \widetilde{H}_b\right)$$

$$C_{ab}^L(\widetilde{H}_a, \widetilde{H}_b) = \frac{\nu_{ab}^D}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial \widetilde{H}_a}{\partial \xi} + \frac{1}{{\rm v}^2}\frac{\partial}{\partial {\rm v}}\left[\frac{\nu_{ab}^{\parallel}}{2}\left({\rm v}^4 \frac{\partial \widetilde{H}_a}{\partial {\rm v}} + \frac{m_a}{T_b}{\rm v}^5 \widetilde{H}_a\right)\right]$$

$$-\widetilde{H}_a k_\perp^2 \rho_a^2 \frac{{\rm v}^2}{4v_{ta}^2}\left[\nu_{ab}^D\left(1+\xi^2\right) + \nu_{ab}^{\parallel}\left(1-\xi^2\right)\right] + R_{\rm mom}(\widetilde{H}_b) + R_{\rm ene}(\widetilde{H}_b)$$

Sonic Transport Fluxes

These are inputs to an independent TRANSPORT CODE

$$\text{particle flux} \quad \Gamma_a = \sum_{\mathbf{k}_\perp} \left\langle \int d^3v \, \widetilde{H}_a^* c_{1a} \widetilde{\Psi}_a \right\rangle$$

$$\text{energy flux} \quad Q_a = \sum_{\mathbf{k}_\perp} \left\langle \int d^3v \, \widetilde{H}_a^* c_{2a} \widetilde{\Psi}_a \right\rangle$$

$$\text{momentum flux} \quad \Pi_a = \sum_{\mathbf{k}_\perp} \left\langle \int d^3v \, \widetilde{H}_a^* c_{3a} \widetilde{\Psi}_a \right\rangle$$

What do we solve for

5-dimensional distribution for every plasma species

Six-dimensional array (mapped into internal 2D array in CGYRO)

$$H_a(\underbrace{k_x, k_y, \theta, \xi, \mathrm{v}}_{\text{5D mesh}}, t)$$

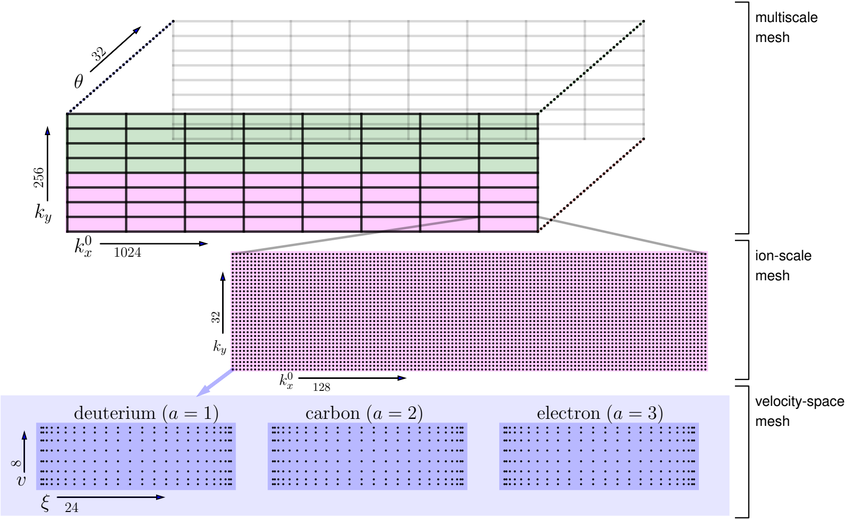
The **spatial coordinates** are

$$\begin{aligned} k_x &\longrightarrow \text{radial wavenumbers} \\ k_y &\longrightarrow \text{binormal wavenumbers} \\ \theta &\longrightarrow \text{field-line coordinate} \end{aligned}$$

The **velocity-space** coordinates are

$$\begin{aligned} \xi = v_\parallel/\mathrm{v} &\longrightarrow \text{cosine of the pitch angle} \in [-1,1] \\ \mathrm{v} &\longrightarrow \text{speed} \in [0,\infty] \ . \end{aligned}$$

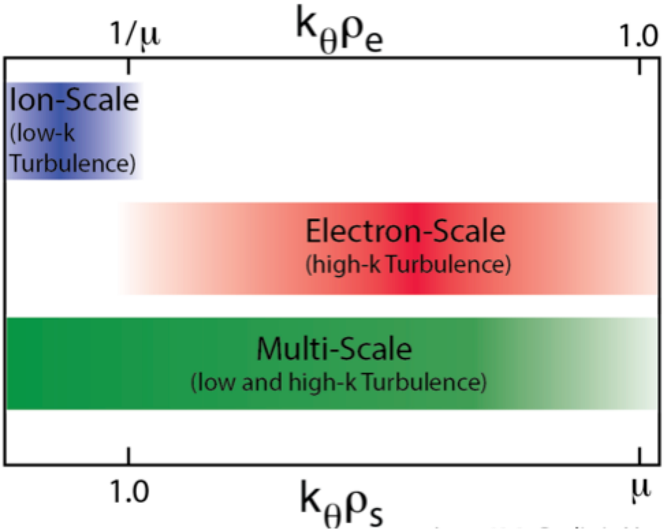
Visual representation of computational mesh



GENERAL ATOMICS

CGYRO optimized for challenging multiscale turbulence

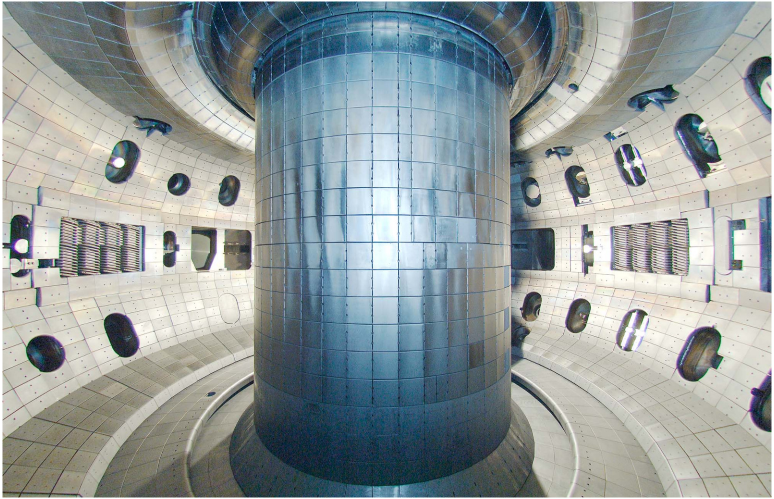
COMPLETE REDESIGN of world-renowned GYRO code



Simulation of turbulent energy loss in a tokamak plasma

CGYRO computes the turbulent flux

DIII-D Tokamak at General Atomics in San Diego, CA



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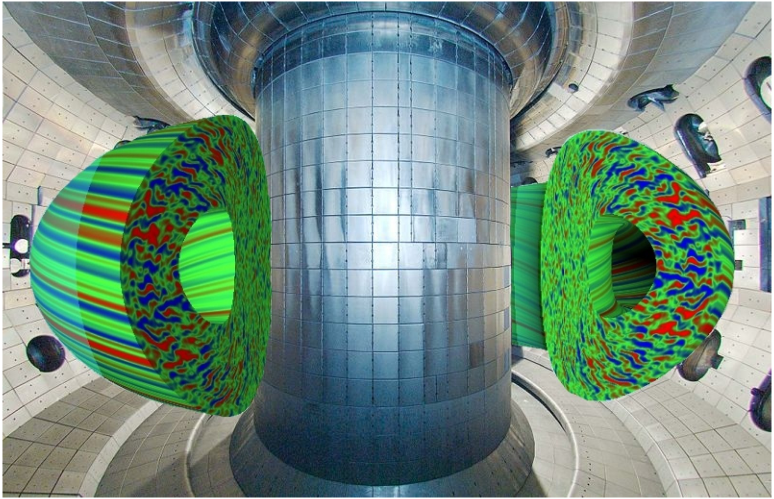

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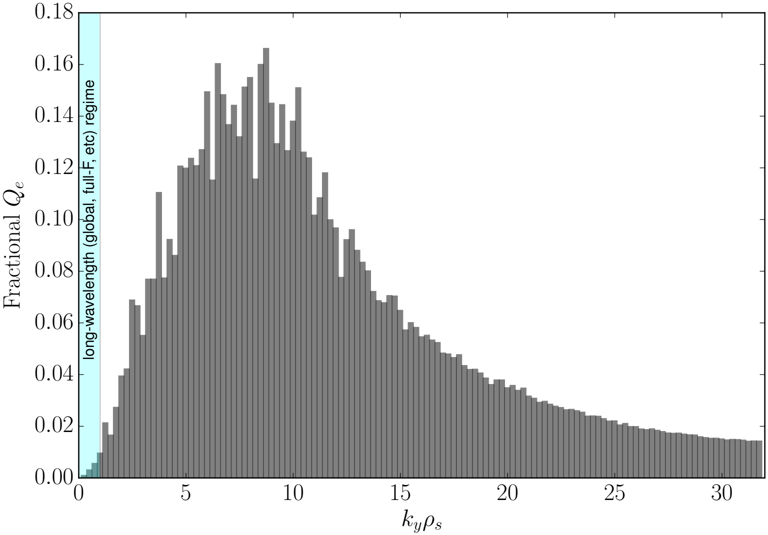
Multiscale DIII-D Simulation at $r/a = 0.92$

ITER baseline discharge (Haskey, Grierson) 164988



Resolution

$k_x\rho_s \leqslant 124.0\,,\quad k_y\rho_s \leqslant 31.8$

Time

9 hrs on 32K cores

	Q_i/Q_{GB}	Q_e/Q_{GB}
pwrbal	2.5	8.2
NEO	2.7	0.0
CGYRO	0.0	8.0

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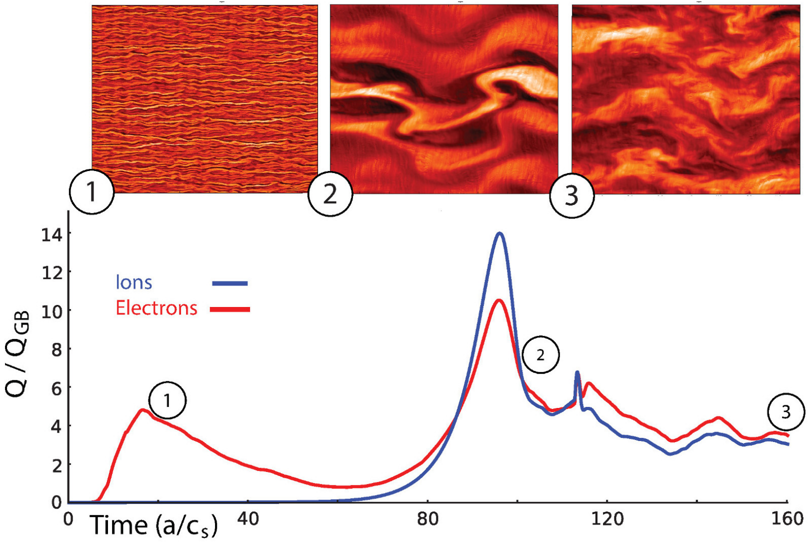
Simulation underway on Titan (NCCS)

4986 nodes = 4986 Tesla K20X GPUs



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Important locations for CGYRO

Source code

`github.com/gafusion/gacode`

DOI

`www.osti.gov/doecode/biblio/20298`

User Documentation

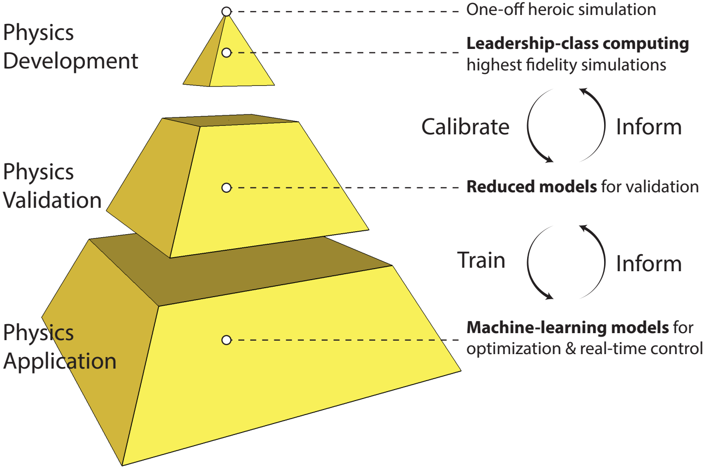
`gafusion.github.io/doc`

Documentary Video (for GYRO)

`www.youtube.com/watch?v=RLI6QW2x4Lg`

Fidelity Hierarchy (Pyramid)

Range of models all the way up to leadership codes



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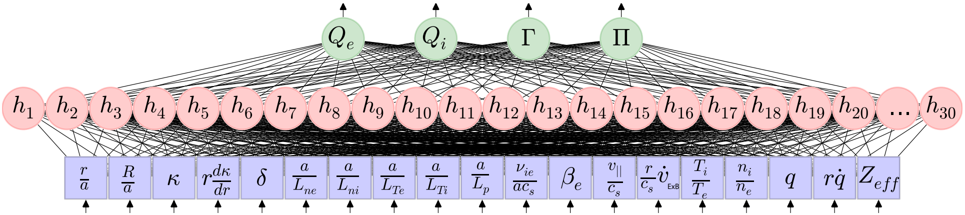
Create TGLF-NN neural net from TGLF reduced model

- **23 inputs** $\rightarrow$ **4 outputs**
- Each dataset has 500K cases from 2300 multi-machine discharges
- Trained with TENSORFLOW
- Must be retrained as TGLF model is updated
- TGLF itself derived from **HPC CGYRO simulation**



GPU performance: development and results

CGYRO: Roadmap for efficient GPU implementation

1. Numerical algorithms selected to allow intensive threading/acceleration
   - Nonlinearity (nl) = FFT
   - Collisions (coll) = Matrix-vector multiply

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   - Smart loop order and good memory management keeps kernels similar

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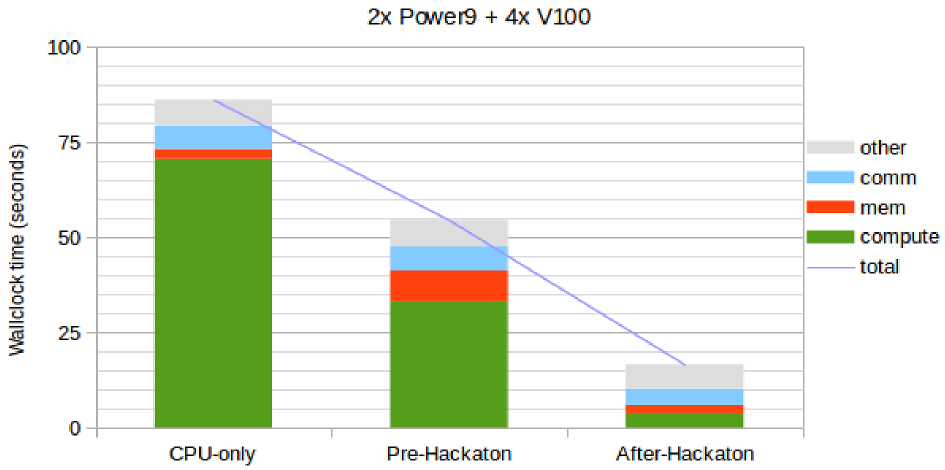
3. Implemented **GPU-aware MPI** (utilizes GPUDirect and GPU-Infiniband RDMA)

Initial thought was that nonlinearity (nl) would dominate



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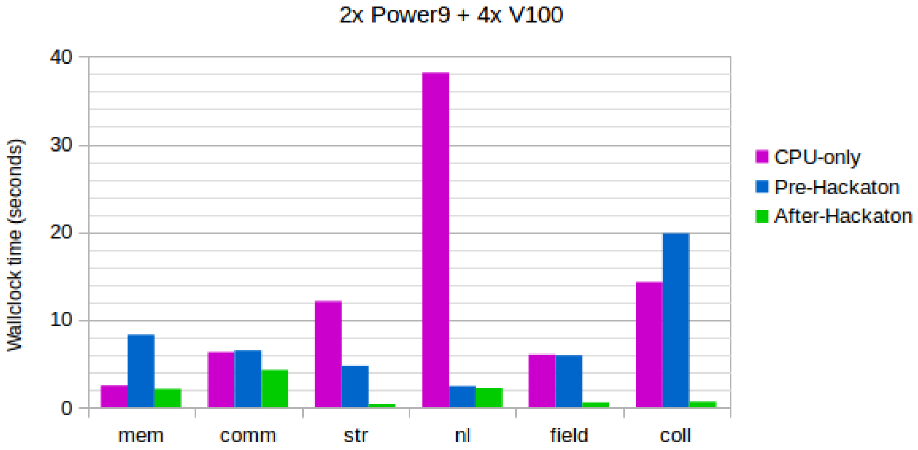
Acceleration of nl exposed cost of other kernels

Titan K20 GPU too small to store collision matrix



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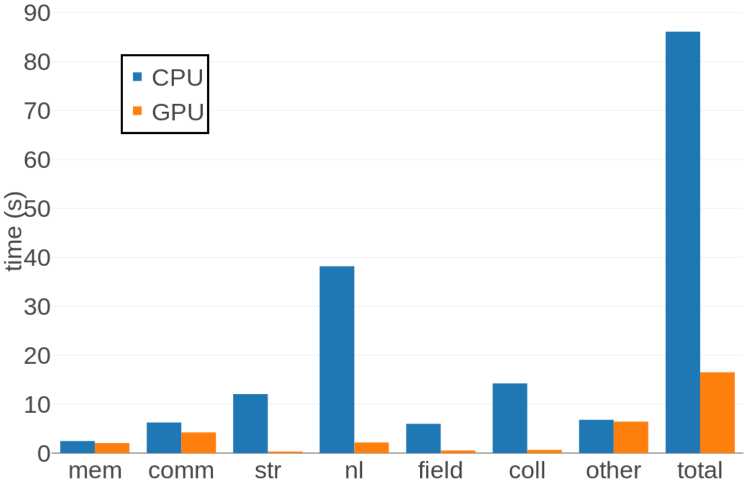
CGYRO: Roadmap for efficient GPU implementation

```
!$acc loop seq
        do ivp=1,nv
           cvec_re = real(cvec(ivp))
           cvec_im = aimag(cvec(ivp))
!$acc loop vector
           do iv=1,nv
              cval = cmat(iv,ivp,ic_loc)
              bvec(iv) = bvec(iv) + cmplx(cval*cvec_re,cval*cvec_im)
           enddo
        enddo
```

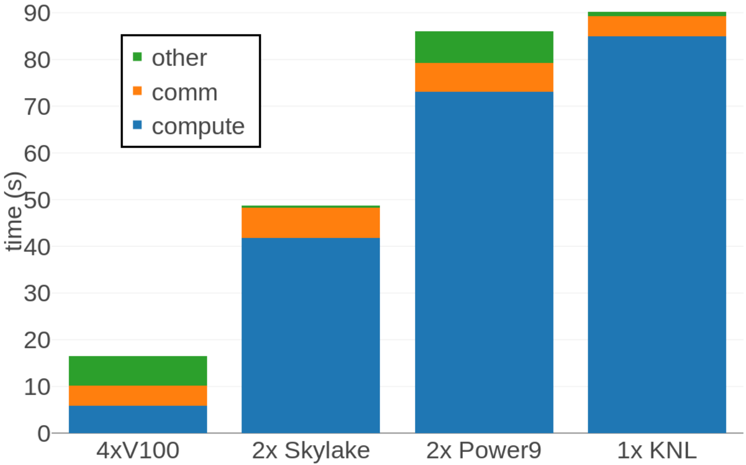
CGYRO: Roadmap for efficient GPU implementation

```
#ifdef DISABLE_GPUDIRECT_MPI
!$acc update host(fsendr)
#else
!$acc host_data use_device(fsendr,f)
#endif
    call MPI_ALLTOALL(fsendr,nsend,MPI_DOUBLE_COMPLEX, &
                      f,     nsend,MPI_DOUBLE_COMPLEX,lib_comm,ierr)
#ifdef DISABLE_GPUDIRECT_MPI
!$acc update device(f)
#else
!$acc end host_data
#endif
```

Power9 (CPU) versus Power9 + 4X V100 (GPU)

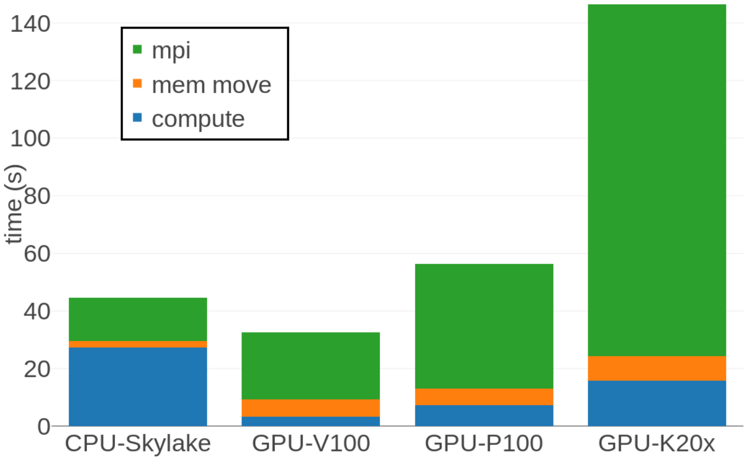


CPU systems versus 4X V100



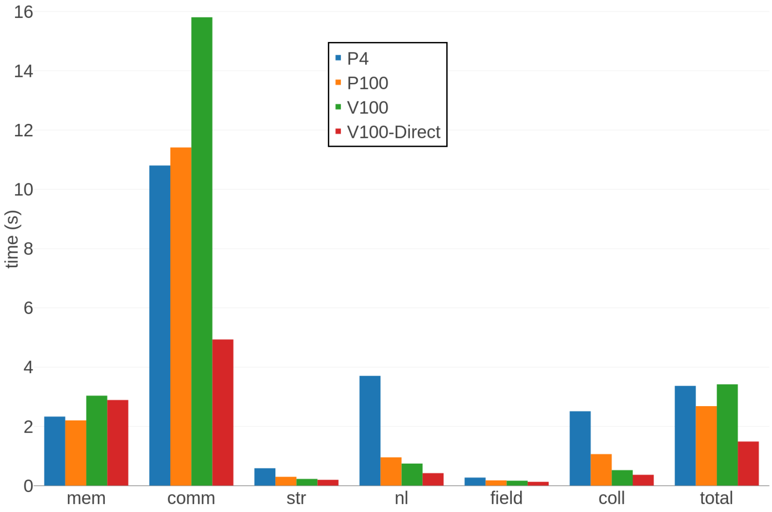
GPU type comparison

Stampede2, GA, Piz Daint, Titan

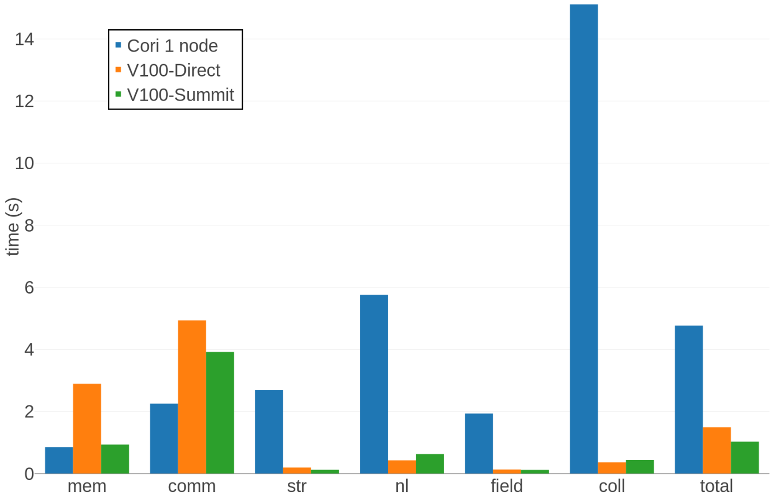


Google Cloud Partition Comparison

Santa Fe (last week)



Cloud V100 compared to Summit and Cori



GENERAL ATOMICS

OUTLINE

1. History of General Atomics?
2. The case for fusion energy
3. Mathematical formulation and GPU-based numerical solution
4. Simulation of turbulent energy loss in a tokamak plasma
5. GPU performance: development and results

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