

# Fermi: What's cooking?

## An overview on some production projects

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## Preliminary remarks:

### Is my application suitable for Fermi?

- a) Does the code use the Message Passing Interface **MPI**?  
(OpenMP is supported only on individual nodes).
- b) Is the **memory requirement per MPI task (less than a) 1 GB (pure MPI) or 16 GB (MPI+OpenMP)?** Is it possible to **exploit SMT technology**?
- c) Is the code **computationally intensive**? That is, is there a small amount of I/O compared to computation? Is the code **floating-point intensive**?
- d) Does the algorithm allow for distributing the work on a **large number of cores**? How does it scale up to with **thousands of threads/tasks**?

## Preliminary remarks: What is Fermi best suitable for?

Largely scalable applications usually imply **LARGE physical problems**, as those dealing with at least one of the following aspects:

- large system size
- high resolution (in space)
- long duration of simulations (or high resolution in time)
- large number or set of interconnected systems or degrees of freedom

# Some examples of research projects on FERMI

A brief overview of a subset of already awarded (and running) PRACE projects:

PROJECT	RESEARCH FIELD	CODE	PROBLEM SIZE	AVERAGE JOB SIZE [N. OF CORES]	BUDGET [M CORE-HOURS]
Euler and Navier-Stokes singularities	Fluid Mechanics	In-house solver	Grid size: $8192^3$ Points: $512 \times 10^9$	32768	50
Artificial Leaf – Shedding light on the catalytic core of artificial leaf technologies	Physical Chemistry	QE	60 atoms+hundreds of water molecules for 20 ps	~10000-30000	33
3D-3V Vlasov simulations of plasma turbulence	Plasma Physics	HVM (Hybrid Vlasov-Maxwell)	Grid points: $128^3$	~20000	25
The way to heating the solar corona: Finely-resolved twisting of magnetic loops	Astrophysics	Pluto	Spatial resolution: 20 km, timestep: $10^{-4}$ s	40000	30
Quantum Monte Carlo simulation of hydrogen at high pressure	Chemistry and Materials	QMCPACK, Turbo-RVB		10000	27
Next generation lattice QCD simulations of the first two quark generations at the physical point	Elementary particles/ QCD	tmLQCD		16384	60

A few words about the project...

## Euler and Navier-Stokes singularities

- **Aim and scientific outcome**: Consolidating our notions on the possible existence of a **finite-time-singularity (FTS) for the Euler and the Navier-Stokes equations**, through extremely large-scale simulations of initial-value problems whereby two Lamb vortex dipoles are made to collide, trying to get as close as possible to the hypothesized FTS, and certainly much closer than previous, lower-resolution studies.
- **Application**: In-house code developed by the applicant which solves the incompressible Navier-Stokes equations discretized on a Cartesian grid with a staggered arrangement of the velocity components. Time advancement is achieved by a hybrid third-order Runge-Kutta/second-order Crank-Nicholson scheme, combined with the fractional-step procedure, with explicit treatment of the convective terms, and implicit treatment of the viscous ones. All spatial derivatives are discretized with second-order central-difference approximations.
- **Additional notes**: It is the **largest simulation** of this kind **ever performed** (grid size:  $8192^3$ , number of points:  $512 \cdot 10^9$ )!

PI: S. Pirozzoli, Sapienza, University of Rome

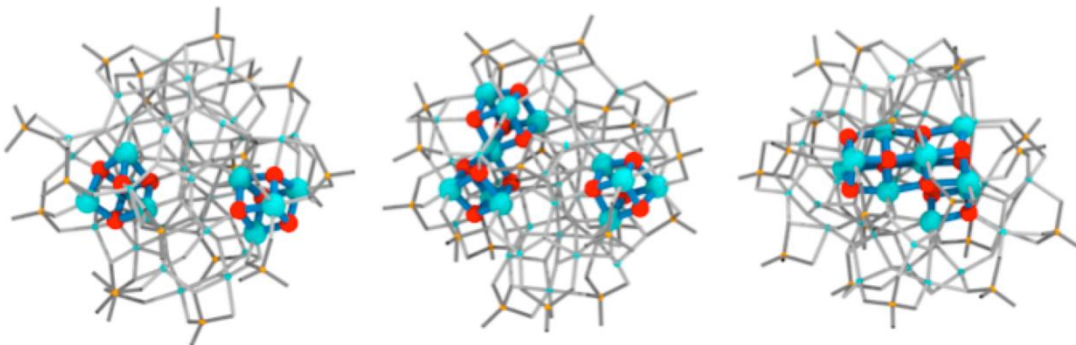
A few words about the project...

## Artificial Leaf :

# Shedding light on the catalytic core of artificial leaf technologies

- **Aim and scientific outcome**: Providing the first realistic and statistically meaningful **structural model of the Co-Pi** (cobalt-phosphate) catalyst, and opening the way for understanding the functionality of catalysts (recently discovered and successfully applied to artificial leaf technologies) in the electrochemical water oxidation reaction, a key photochemical reaction in solar fuel production. If successful, the study will provide useful guidelines for the rational design of superior catalysts for the direct conversion of solar energy into fuels.

- **Application**: Quantum Espresso
- **PI**: S. Fabris, CNR-IOM DEMOCRITOS and SISSA



*First realistic model structures of the Co-Pi catalyst identified by recent computational modeling based on ab-initio metadynamics*

A few words about the project...

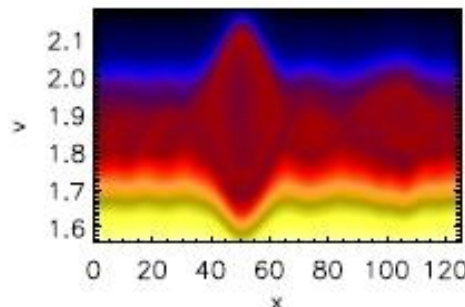
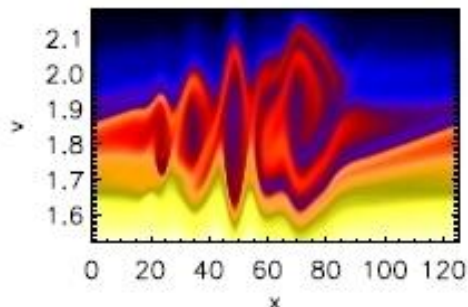
## 3D-3V Vlasov simulations of plasma turbulence

- **Aim and scientific outcome**: Studying of **turbulence and magnetic reconnection** in space plasmas to the full dimensional 3D-3V phase space configuration and analysing of the role of kinetic processes at play in the turbulent cascade in the **solar wind**, its relationship with explosive magnetic reconnection events and the evolution of the distribution of particle velocities. Results of these massive simulations are expected to provide crucial information on the local heating of the solar wind and in the interpretation of in situ measurements from spacecraft.

**Application**: HVM (Hybrid Vlasov-Maxwell), developed by the applicant, which integrates the Vlasov equation for the distribution function in phase space coupled to an algorithm for the integration of the Maxwell equations. It uses an Eulerian approach consisting in discretizing the equations on a fixed in time space-velocity grid.

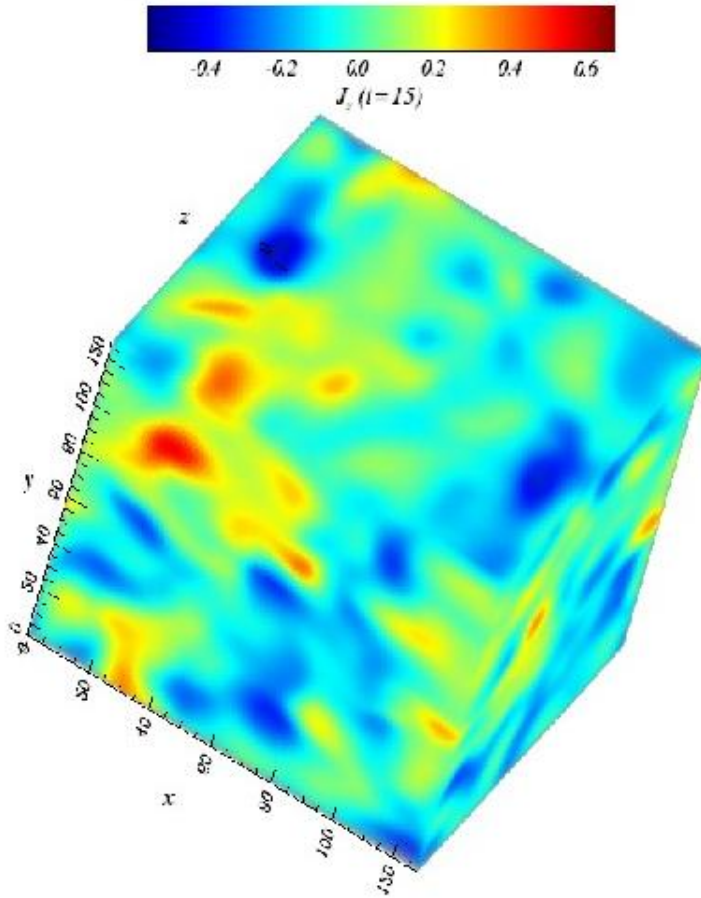
- **Additional note**: The first and unique (to date) attempt to provide a realistic interpretation of experimental measurements in space.

- **PI: F. Valentini, Calabria University**

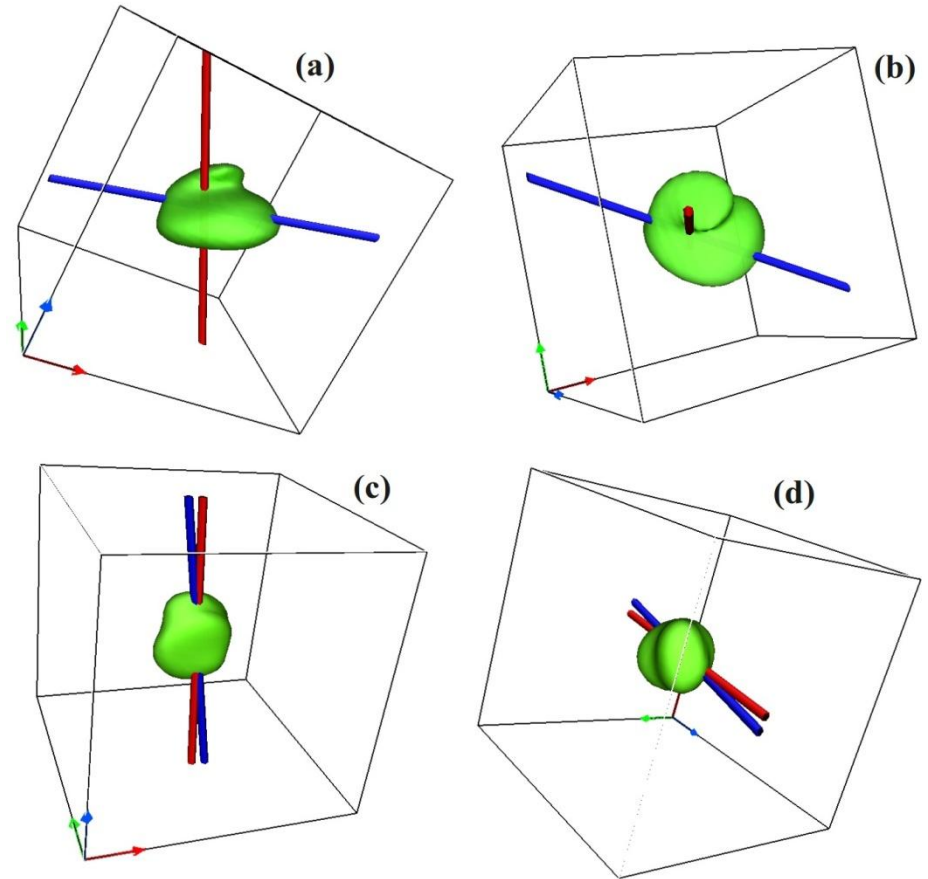


Proton distribution function in the  $x$ - $V_x$  phase space at two different times.

## Preliminary results



Current density while turbulence sets up.



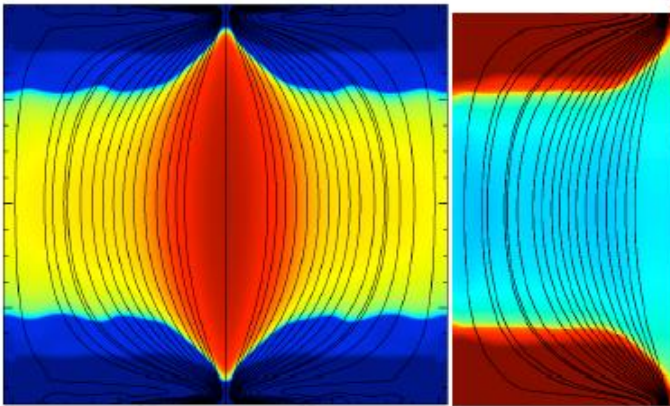
Iso-surfaces of velocity distribution function for solar wind ions.



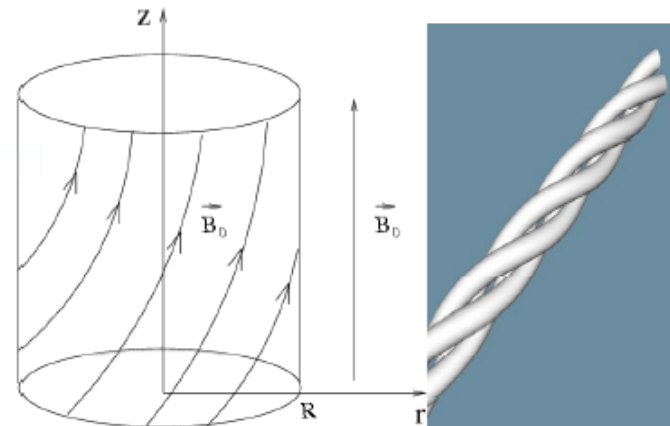
A few words about the project...

## The way to heating the solar corona: Finely-resolved twisting of magnetic loops

- **Aim and scientific outcome:** Studying the twisting of coronal loops with unprecedented model (ten-fold) resolution and completeness, necessary to answer reliably and for the first time important questions on coronal heating, e.g., how is reconnection distributed along and across the loop? How does it compete with kink instability? Does it reach a steady state?
- **Application:** Pluto
- **PI:** F. Reale, University of Palermo



*Temperature map and magnetic field lines (left) of a cross-section of the 3D domain; density map (right) for 2D simulation.*



*Sketch of the twisted magnetic field.  
Twisted and tangled magnetic flux tubes.*

A few words about the project...

## Quantum Monte Carlo simulation of hydrogen at high pressure

- **Aim and scientific outcome:** Applying first principles simulation methods (based on quantum Monte Carlo and density functional theory) to elucidate the equilibrium properties and to explore superconductivity of hydrogen at high pressure, which is of interest in astrophysics (e.g. for the giant planets and the recently observed exoplanets) and for technological reasons such as for experiments conducted at the National Ignition Facility at the Lawrence Livermore National Laboratory.
- **Applications:** QMCPACK (implements various QMC algorithms, including correlated sampling techniques using VMC and Reptation methods, and employs multi-level parallelizations using hybrid OpenMP/MPI), Turbo-RVB(uses linear algebra routines (lapack-scalapack-essl)), QE.

PI: C. Pierleoni, University of L'Aquila

A few words about the project...

## First Lattice QCD study of B-physics with four flavors of dynamical quarks

**Aim and scientific outcome:** Extensive study of B-physics based on Lattice QCD, addressing issues which are relevant for the phenomenology of the Standard Model (SM) as well as for its most general New Physics (NP) extensions, that are currently under investigation by the LHCb experiment and will be studied also at the planned super B-factories.

**Application:** tmLQCD

PI: S. Simula, INFN

A few words about the project...

## Next generation lattice QCD simulations of the first two quark generations at the physical point

**Aim and scientific outcome:** generation of gauge field configurations with all quarks of the first two generations having their physical masses. These simulations are complemented by computations with four degenerate quark flavors needed for the renormalization program.

**Application:** tmLQCD

PI: K. Jansen, NIC, DESY Zeuthen