POLITECNICO DI MILANO

High Performance Computing:
tecnologia abilitante per la Ricerca e per l'Innovazione





LISA come piattaforma abilitante per il Politecnico di Milano

Prof. Fabio Inzoli
Dipartimento di Energia - Politecnico di Milano

Sommario

- Introduzione
- LISA e Politecnico di Milano
- LISA e Dipartimento di Energia
- Conclusioni

HPC come **strumento**

HPC come **condizione** necessaria **per competere**

HPC come **opportunità**

Dipartimenti coinvolti (LISA 2013-2014)

- Scienze e Tecnologie Aerospaziali
- Energia
- Chimica, Materiali e Ingegneria Chimica
- Ingegneria Civile e Ambientale
- Ingegneria Matematica
- Meccanica
- Elettronica, Informatica e Bioingegneria
- Architecture, Building and Construction

36.6 Mh

Ambiti

- Aerospazio
- Energia
- Materiali
- Ambiente
- Biotecnologie
- Automotive

Progetti (LISA 2013-2014)

- **CHILDHOOD** energia
- **CREAM** energia
- **CORE** energia
- **FBI** materiali
- **LAPLAST** energia
- ……

Title: *LAser-PLasma Acceleration with Structured Targets*

Research Group

• Andrea Sgattoni (PI)	*Politecnico di Milano (now CNR-INO Pisa)*
• Matteo Passoni	*Politecnico di Milano*
• Lorenzo Cialfi	*Politecnico di Milano*
• Andrea Macchi	*CNR-INO Pisa*
• Luca Fedeli	*Università di Pisa*
• Stefano Sinigardi	*Università di Bologna*

Period: *May 2014 – May 2015*

Hours @ FERMI: *about 3.000.000*

Scientific Aims

the main program of this project is to study *fundamental aspects of the physics of the interaction of superintense laser with solid targets and related particle acceleration mechanisms*.

Potential Scientific & Industrial Impact

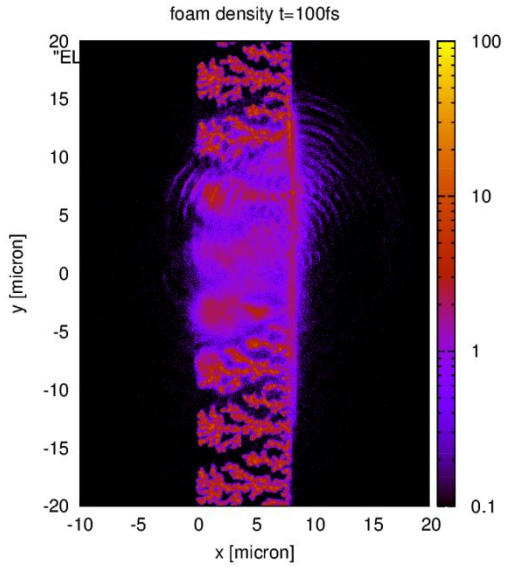
Obtain major scientific advances to support the achievement, in the next future, of:

- new particle acceleration technologies

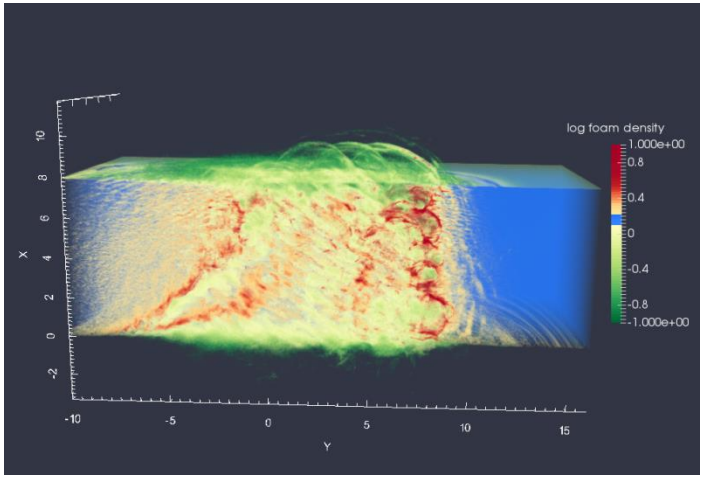
- interest of such novel accelerators in the medical field (e.g. radioisotopes production for diagnosis and treatment), materials (material irradiation, characterization, processing) and nuclear engineering (e.g. novel scheme of inertial fusion and investigation/exploitation of exotic radionuclides).

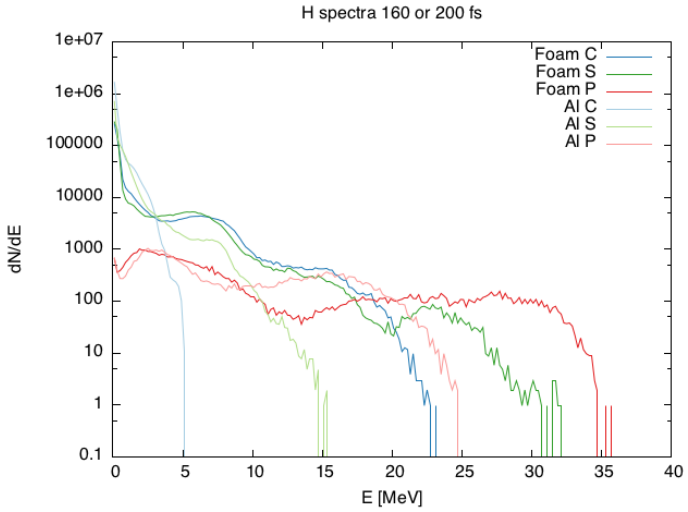
- *These subjects will be further developed, at POLIMI, also thanks to an approved ERC Co Grant (ENSURE, PI Matteo Passoni).*
- *Further access to CINECA strongly required in the next years!*

Current activity & preliminary results



Work in progress!





- Development of 2D-3D kinetic simulations of laser-matter interaction with complex targets
- Development and benchmark of novel codes

Research Group:

- Dr. Elena Macerata, Principal Investigator
- Prof. M. Mariani
- E. Mossini, Ph.D. Student
- M. Cerini, Ph.D. Student

- Dept. of Energy, Radiochemistry and Radiation Chemistry Laboratory

- Prof. E. Padovani
- Prof. F. Giacobbo

- Dept. of Energy, Contaminants Migration and Safeguard Laboratory

- Prof. C. Cavallotti

- Dept. of Chemistry, Materials and Chemical Engineering

LISA Production project call 1

Chemical issues in Lead Fast Reactors by theoretical methods - CHILDHOOD

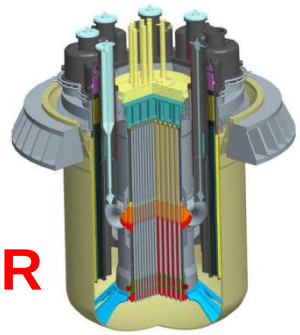
- 12 months (May 2013 – April 2014)
- Budget: 94000 std hours on EURORA, PLX, FERMI

LISA Development project

Computational approach for fuel-coolant chemical compatibility in Lead-cooled Fast Reactors - FueLead

- 6 months (June 2014 – December 2014)
- Budget: 50000 std hours on PLX

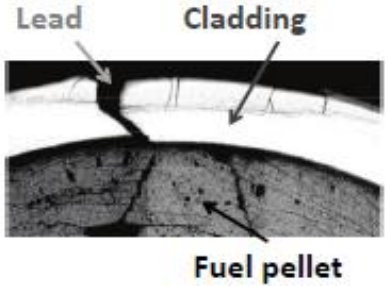
Within the development of **Gen IV Lead-cooled Fast Reactors**



LFR

arising from the idea to exploit the computational chemistry potentialities in a field such as the nuclear area, where the experiments are often difficult, hazardous and expensive,

the **CHILDHOOD and FueLead projects** would like to contribute to acquire information about the **chemical interaction between irradiated nuclear fuel and liquid lead** in the event of cladding failure.



⇒ by developing a theoretical approach based on Density Functional Theory
⇒ by applying sistematically the method to study species that could be formed by the chemical interactions in order to provide estimations of unknown thermochemical data
⇒ by studying the composition of the fuel-coolant system at thermodynamic equilibrium with such thermochemical data

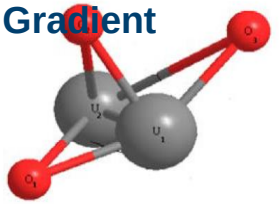
Main Results

Development of an approach based on Density Functional Theory – Generalized Gradient Approximation by Gaussian09 code for gas phase

- by evaluating different functional/basis-set combinations
- by choosing suitable testing parameters
- by checking the chosen approach by comparison with two well-established functionals (B3LYP and M06)
- validation by comparison with experimental data

U_2O_3

Equilibrium structure



Multiplicity	Energy [Hartree]	Distance U_1-O [nm]	Distance U_2-O [nm]	Distance U_1-U_2 [nm]	Angle U_2-O_2-U_1
5	-1179.95647153	0.20915	0.21116	0.295881	89.487°
7	-1179.97593918	0.21090	0.21167	0.297699	89.577°
9	-1179.85350763	0.21485	0.21619	0.318438	92.342°

Application of the method to several compounds of interest for the application

- Estimation of unknown data

Molecule	Vibrational Frequency [cm^{-1}]		Entropy [J/K·mol]		Specific Heat Capacity [J/K·mol]		Formation Enthalpy [kJ/mol]	
	Calculated	Experimental	Calculated	Experimental	Calculated	Experimental	Calculated	Experimental
UO_2	807.8	820.0	251.013	263.554	47.022	51.347	-565.0	-477.8
UO_3	904.7	852.5	309.644	308.683	63.575	64.542	-892.1	-799.2
PuO_2	832.6	786.8	275.951	278.0 ± 5	46.501	-	-373.2	-410.2
UPb	93.3	-	295.341	-	37.272	-	501.6	-
UPb_3	135.6	-	444.145	-	82.277	-	88.9	-
PuPb	87.7	-	297.267	-	37.292	-	478.9	-
PbO	764.9	721.0	239.536	240.039	32.072	32.510	-84.5	70.2

Results Dissemination

M. Cerini, G. Dia, E. Macerata, E. Mossini, M. Giola, M. Mariani, C. Cavallotti, *Proc. Int. 23rd International Conference Nuclear Energy for New Europe-NENE 2014, Portorose, Slovenia, Settembre 8-11, 2014, p. 1209, Nuclear Society of Slovenia (2014) (CD-ROOM), ISBN 978-961-6207-37-9*
M. Cerini, E. Macerata, M. Giola, M. Mariani, C. Cavallotti, *Advancing the chemistry of the f-elements, Dalton Discussion 14*, 28-30 July 2014, Edinburgh, UK

Main Results

Evaluation of solubility of gaseous fission products in liquid Pb

- by Polarizable Continuum Model within DFT-GGA with the plane wave pseudopotential method included in Gaussian09

Element in liquid Pb		O	I	Kr	Xe
Solubility [g/L*100]	calc	3.183	39.456	12.677	19.967
	exp	3.807	-	-	-

DFT-GGA approach by VASP (*Vienna Ab-initio Simulation Package*) code for cristalline phase

Molecule	Entropy [J/K·mol]		Specific heat capacity [J/K·mol]	
	Calculated	Experimental	Calculated	Experimental
UO_2	80.20	77	63.71	63.57
PuO_2	82.37	66	64.31	66.25
AmO_2	80.06	67	65.96	66.17
$BaUO_3$	160.26	149.1	113.96	110.36
$LaPb_3$	172.63	-	103.73	-
$SrPb_3$	170.61	-	103.13	-
UPb_3	164.15	-	102.19	-
Pu_3Pb	172.73	-	103.76	-

Results Dissemination

M. Cerini, E. Macerata, M. Giola, M. Mariani, C. Cavallotti, *DFT-GGA Predictions of Thermodynamic Parameters in Solid Phase for Binary Compounds of Actinides and Fission Products*, GLOBAL 2015 International Conference, 20-24 September 2015, Paris, France

All these information are fundamental in order to:

- **create a Database** of thermodynamic parameters available for researchers in nuclear field
- **foresee the evolution of an incidental event** with contact between irradiated fuel and liquid Pb
- **assess the safety** of such kind of reactor concept
- **plan suitable actions** to avoid damages to the reactor and to preserve workers and public from health risks

The computational approach proposed could be an effective tool for preliminary evaluations of chemical systems as well as to support experimental activities.

Title: *Advanced microreactor modeling for energy and environment.*

Research Group

- Matteo Maestri (PI) — *Dept. Energy*
- Andrea Sgattoni — *Dept. Energy*
- *Alberto Cuoci* — *CMIC*

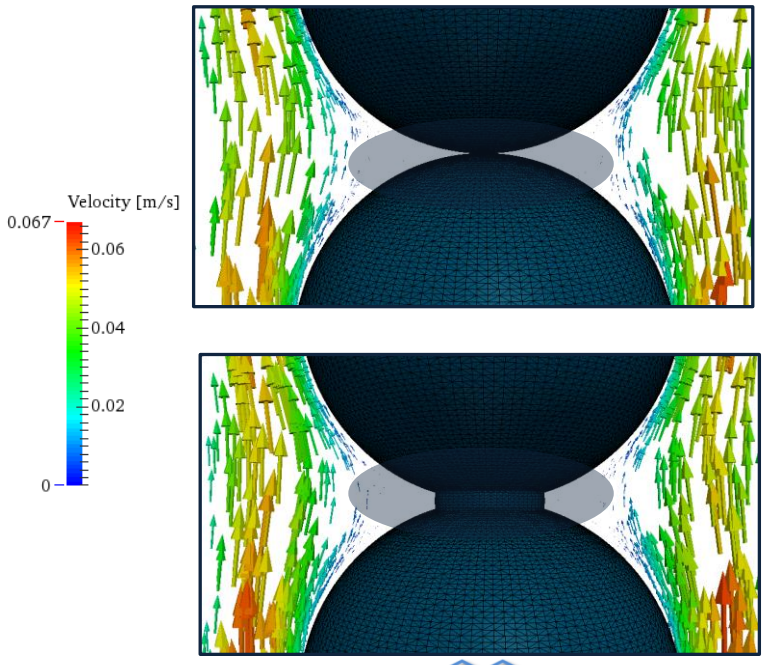
Period: *November 2013 – November 2014*

Hours: *about 3.000.000*

Goal and main results

- ✓ Detailed understanding of interaction between chemistry and transport in microcreators for energy and environment
- ✓ Detailed study on the effect of meshing contact points and its effect on the simulated surface reactivity

Code: CatalyticFOAM



Publications:
S. Rebughini, A. Cuoci, M. Maestri, Ind. Eng. Chem. Res., 2015

CatalyticFOAM

Title: *First-principles assessment of uBI-method for microkinetic modeling of catalytic processes*

Research Group

- Matteo Maestri (PI) — *Dept. Energy*
- Luca Dietz — *Dept. Energy*
- *Filippo Motta* — *Dept. Energy*

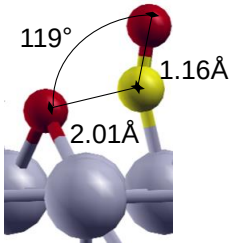
Period: *May 2014 – May 2015*

Hours: *about 3.500.000*

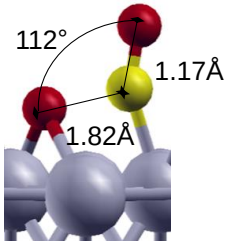
Goal and main results

- ✓ Atomistic study of the mechanism of elementary catalytic reactions
- ✓ Identification of global parameters and descriptors of the catalytic activity for catalyst design
- ✓ Validation of UBI semiempirical method

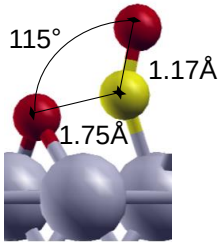
Code: Quantum Espresso



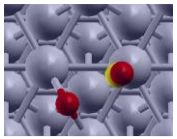
Pt (111)

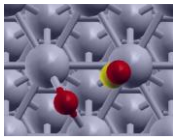


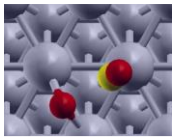
Rh (111)



Ni (111)







$CO_2 \rightarrow CO + O$

Publications:

L. Dietz, S. Piccinin, M. Maestri, Journal of Physical Chemistry C, 119 (2015) 959–4966

LISA e Dipartimento di Energia
MSFR

Title: Molten Salt Fast Reactor

Research Group

- *Antonio Cammi (PI)* — *Dept. Energy*
- *Luca Aufiero* — *Dept. Energy*
- *Marco Ricotti* — *Dept. Energy*

Period: *November 2013 – November 2014*

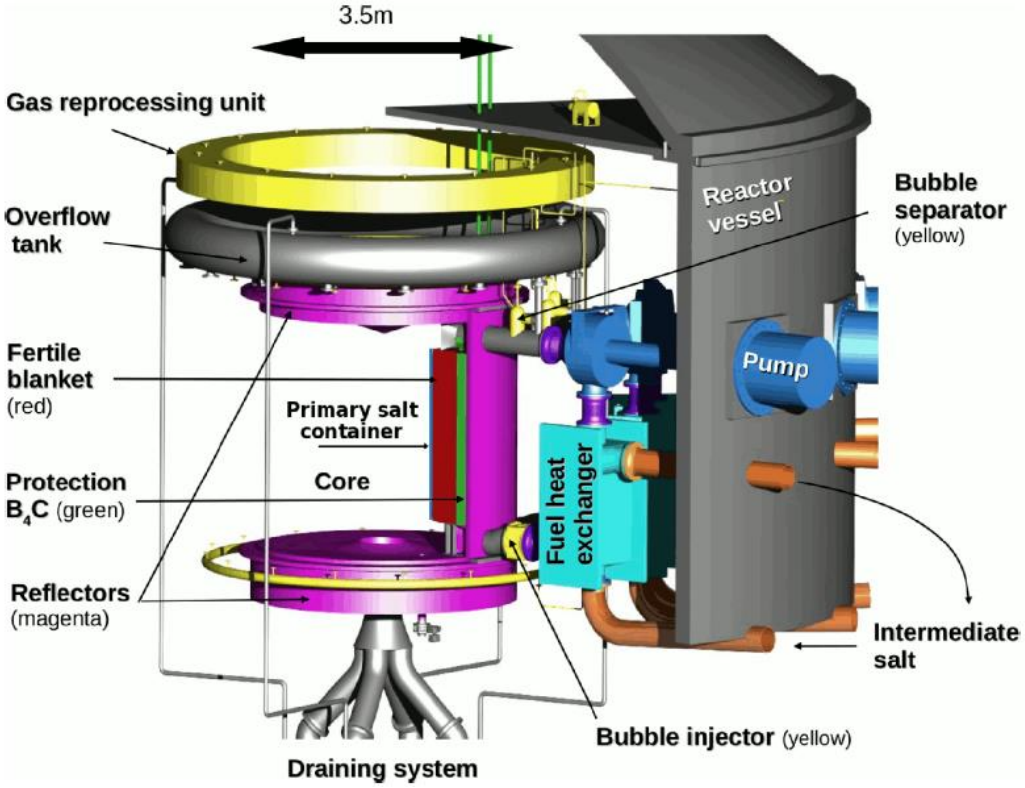
Hours: *about 500.000*

Publications:

M. Aufiero, M. Brovchenko, A. Cammi, I. Clifford, O. Geoffroy, D. Heuer, A. Laureau, M. Losa, L. Luzzi, E. Merle-Lucotte, M.E. Ricotti, H. Rouch - Calculating the effective delayed neutron fraction in the Molten Salt Fast Reactor: Analytical, deterministic and Monte Carlo approaches, Annals of Nuclear Energy – Vol 65, March 2014, pp 78-90.

LISA e Dipartimento di Energia
MSFR

The Molten Salt Fast Reactor (MSFR) is the reference circulating-fuel reactor in the framework of the Generation IV International Forum.



The reactor is designed to operate in the Th/^{233}U fuel cycle with a fast-to-intermediate neutron spectrum and a nominal thermal power of 3 GW.

Monte Carlo-based **fuel cycle analysis**:

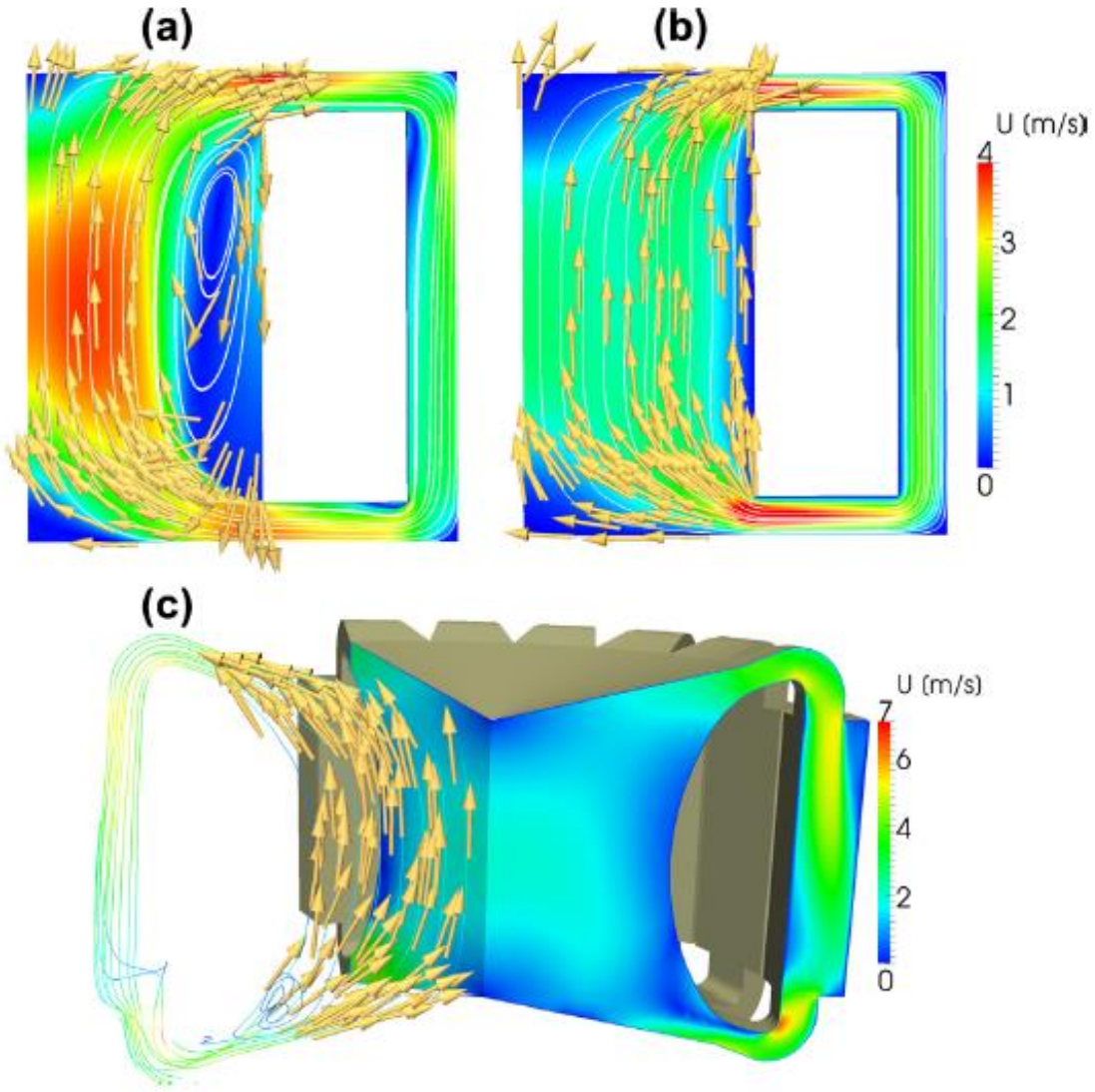
- on-line reprocessing and reactivity control

Coupled **neutronics-CFD** simulations:

- Consistent and efficient coupling and time-integration techniques

Adjoint-weighted **calculations in circulating-fuel reactors**:

- Monte Carlo and deterministic approaches



Conclusioni

Volevo segnalarti che noi abbiamo usufruito del bando Lisa, in particolar modo con il dottorando Manuele Aufiero, ricevendo un utilissimo supporto per l'ottimizzazione delle opzioni di compilazione di Serpent (un codice di neutronica) su FERMI.

Il referente per il nostro progetto è stato molto gentile e disponibile, ci ha permesso di utilizzare Serpent in maniera ottimale su Fermi.

Senza questo supporto non avremmo potuto ottenere i risultati che abbiamo raggiunto.

Nelle scorse settimane ci hanno finanziato un progetto nell'ambito di H2020

Collaborazione + interdisciplinarietà = competitività