The QCD critical point via Padé and multi-point Padé resummations (EHPC-EXT-2022E01-055)

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HotQCD Collaboration:
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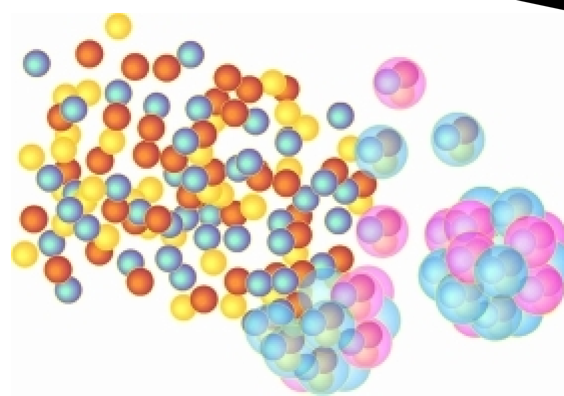
[PRD 105 (2022) 7, 074511, arXiv: 2202.09184]

Bielefeld Parma Collaboration:
David Clarke, Petros Dimopoulos, Francesco Di Renzo, Jishnu Goswami, Guido Nicotra, CS, Simran Singh, Kevin Zambello
[PRD 105 (2022) 3, 034513, arXiv: 2110.15933]

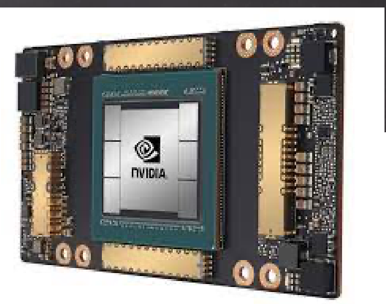
Brussels, December 11, 2023

What is it all about :

Nuclear physics:
quarks vs. hadrons

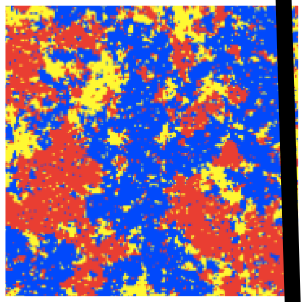


HPC



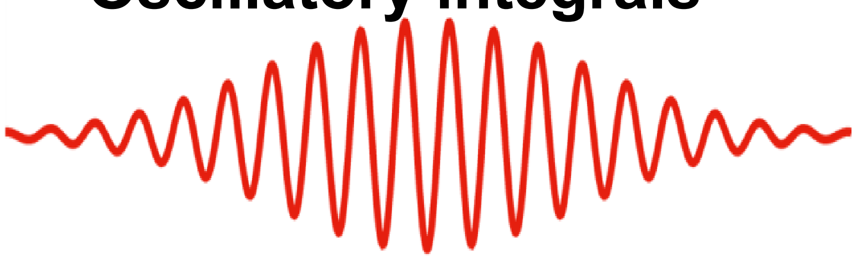
Lattice QCD at nonzero temperature

Thermodynamics and statistical physics:
- Equation of state
- phase transitions
- critical phenomena

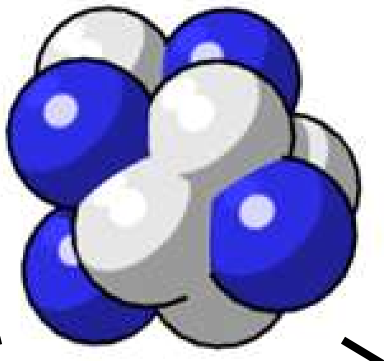


Heavy ion collisions:
- Nucleus-nucleus collisions at LHC and RHIC

Algorithms:
- Large and sparse matrices
- Oscillatory integrals

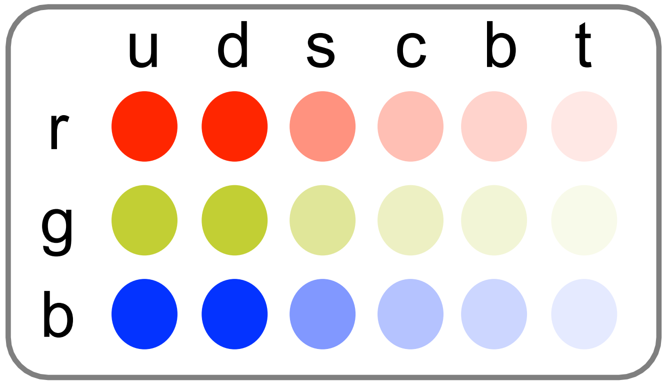


Fundamental building blocks of matter:

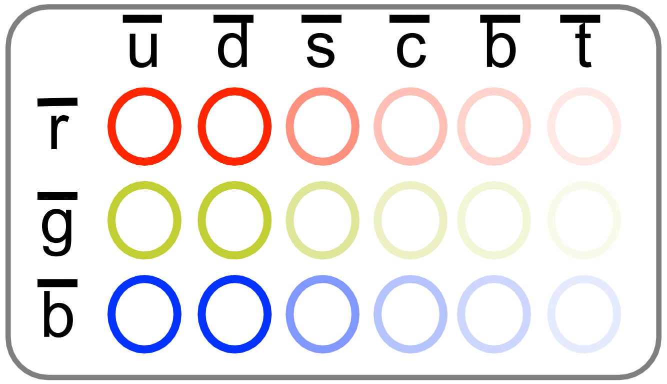
Electro-magnetism	Weak interaction	Strong interaction	Gravity
			

QCD: Quantum Chromodynamics

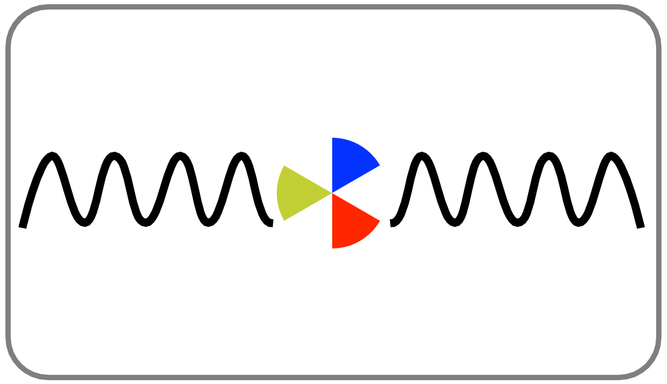
Quarks



Anti-quarks



Gluons



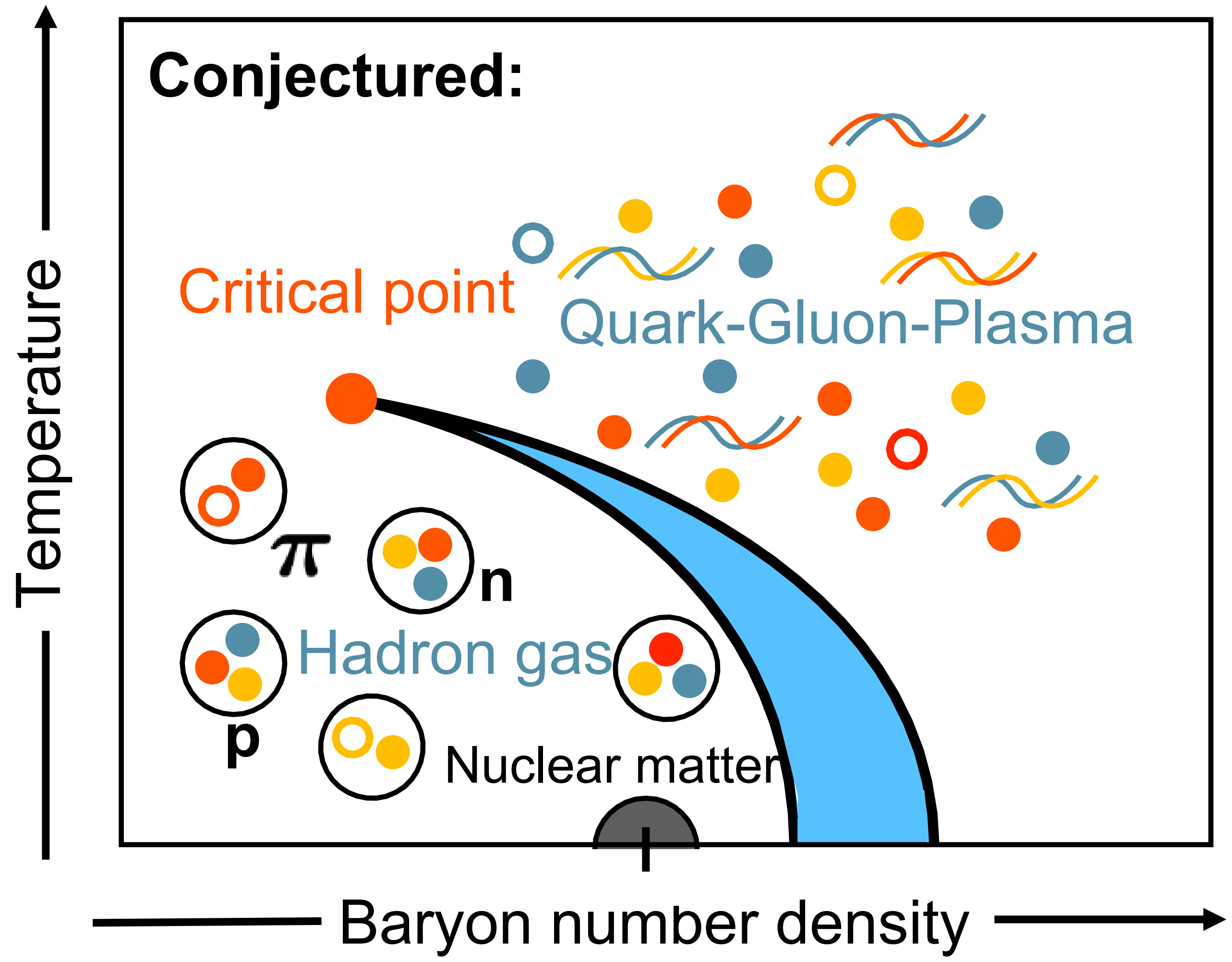
1960-1964 M. Gell-Mann, G. Zweig, introducing the quark model

Nobel price 1969: M. Gell-Mann

The phase diagram of QCD

- QCD thermodynamics is a consequence of **spontaneous chiral symmetry breaking** and **liberation of new degrees of freedom: quarks**

- The QCD phase diagram is encoded in the **QCD partition function** and can be calculated by **lattice QCD** at small baryon number density.



The QCD phase diagram

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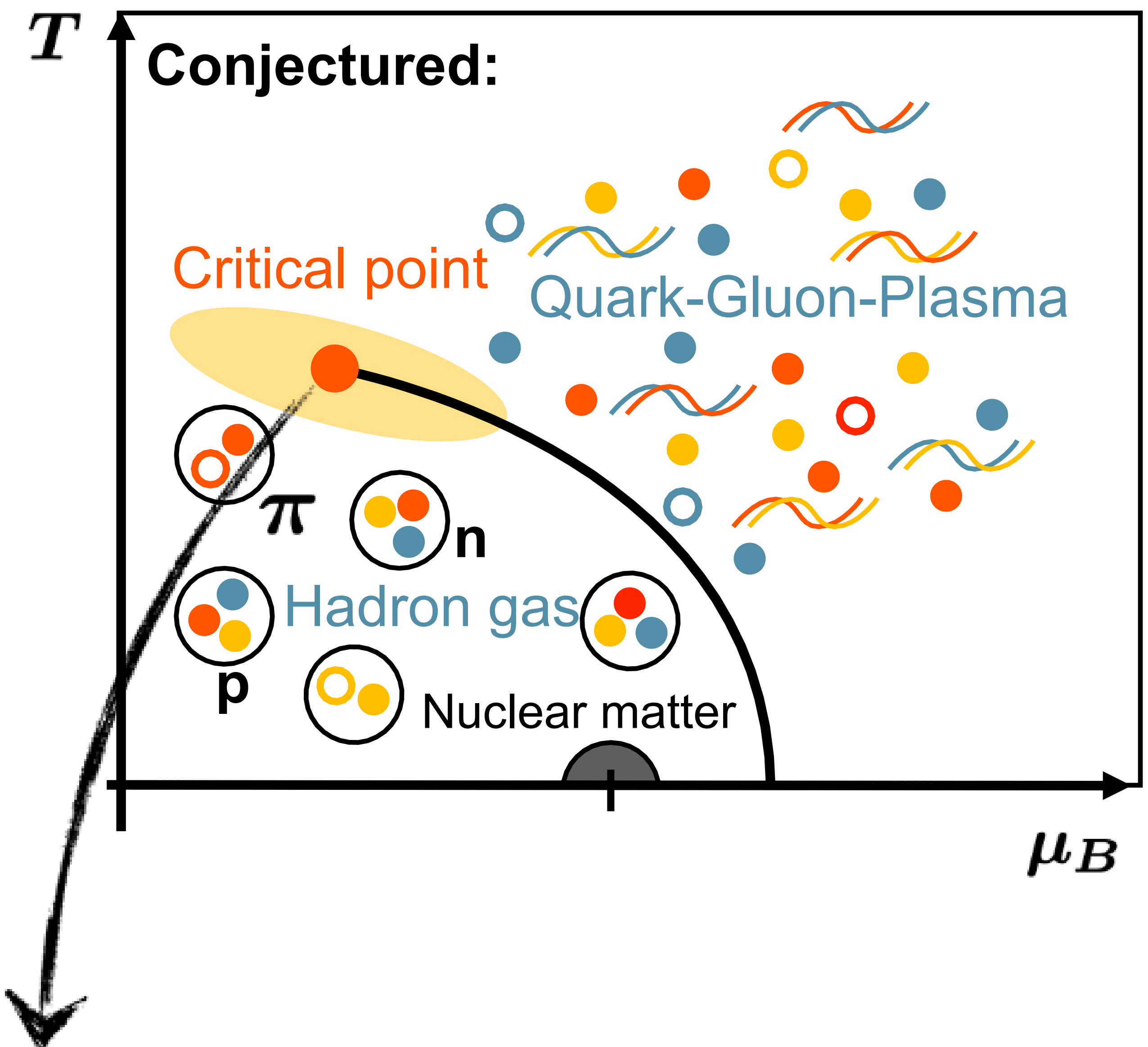
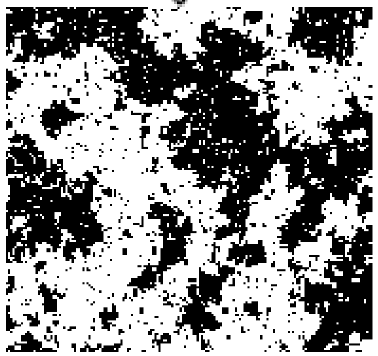
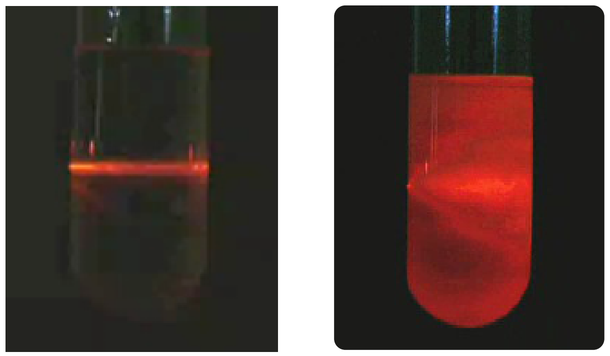
- The QCD phase diagram is encoded in the **QCD partition function** and can be calculated by **lattice QCD** at small baryon number density.

- Important Landmark: A (conjectured) **critical point**, giving rise to a diverging correlation length and universal scaling.





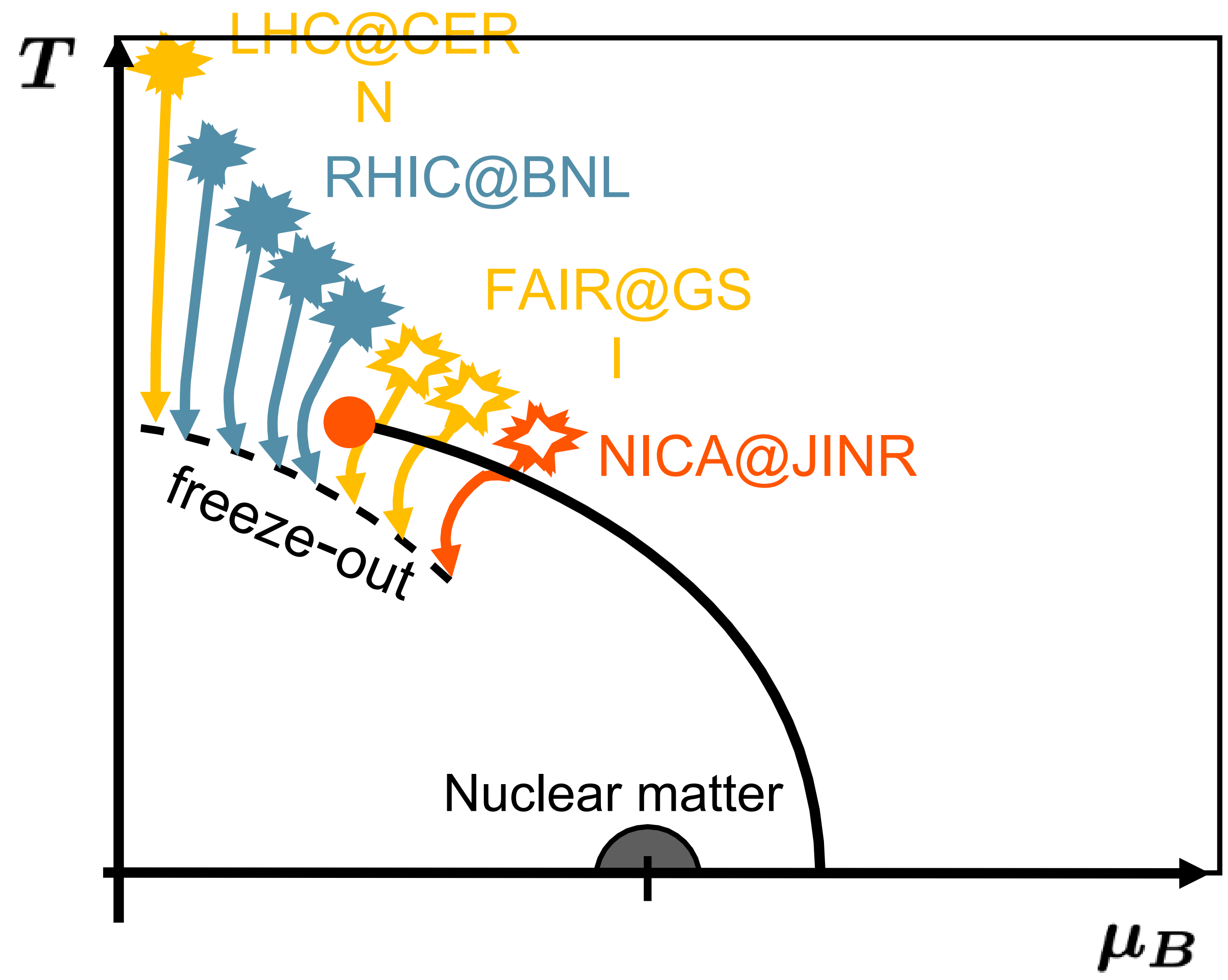
Critical fluctuations of the 3d-Ising model



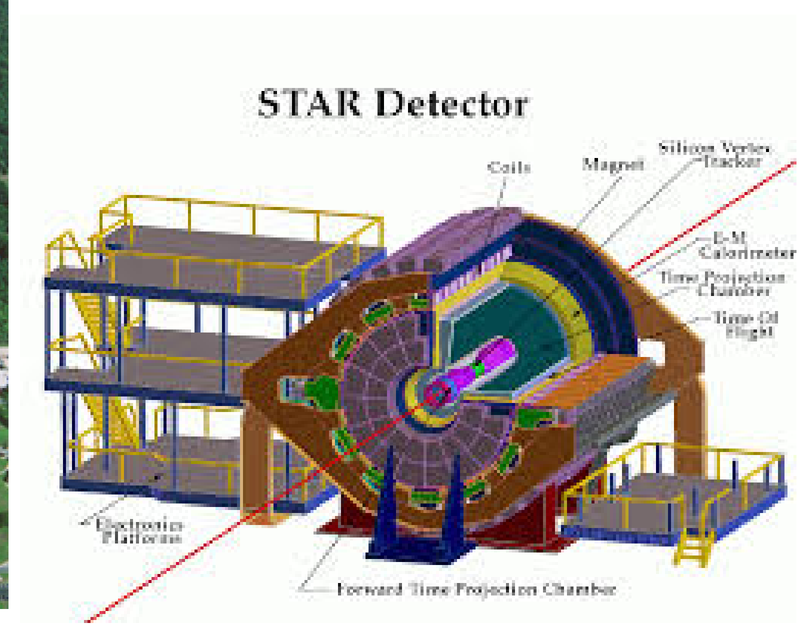
Critical opalescence in water

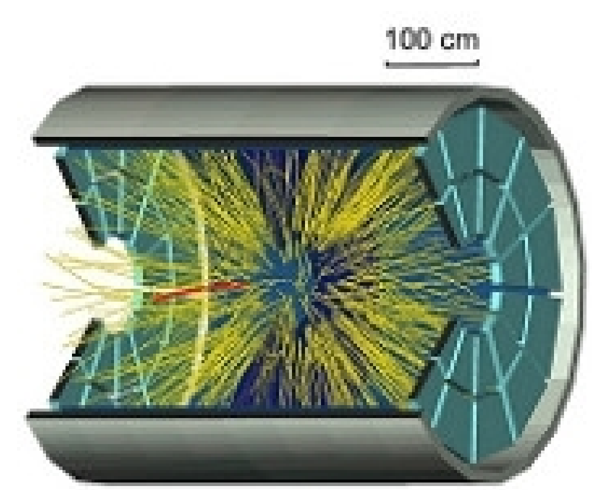
The QCD phase diagram

- The **early universe** passed the QCD phase transition (at small baryon number density).
- The QCD phase diagram is studied in nucleus-nucleus collisions. In particular the “Beam Energy Scan” program at RHIC is partly motivated by the search for the QCD critical point.



Relativistic Heavy Ion Collider at BNL

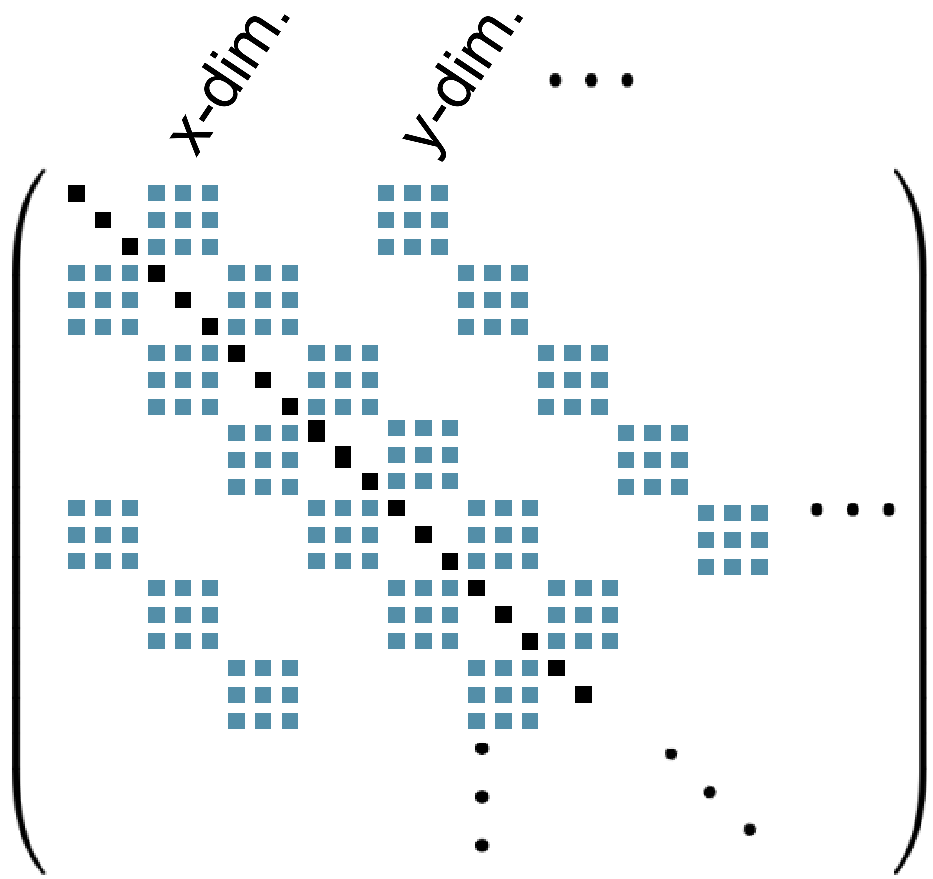




Lattice QCD

- The QCD partition function as path integral:

$$Z(T,V,\mu) = \int \left(\prod_{x,\mu} \mathrm{d}\bar{\psi}_x \,\mathrm{d}\psi_x \,\mathrm{d}U_{x,\mu}\right) e^{-\bar{\psi}_x M_{xy}(U)\psi_y - \beta S_G(U)}$$
$$= \int \left(\prod_{x,\mu} \mathrm{d}U_{x,\mu}\right) \det M(U)\, e^{-\beta S_G(U)}$$

$M =$ 

Fermion matrix: large, sparse, band structure is induced by the discretisation of the kinetic terms (derivative), the discretisation is improved by smearing and next-to-next-to nearest interactions

Hybrid Monte Carlo Integration:
$\approx 10^6$ lattice points
$\approx 10^8$ degrees of freedom

- The QCD partition function as path integral:

$$Z(T,V,\mu) = \int \Big(\prod_{x,\mu} \mathrm{d}\bar{\psi}_x \, \mathrm{d}\psi_x \, \mathrm{d}U_{x,\mu}\Big) \, e^{-\bar{\psi}_x M_{xy}(U) \psi_y - \beta S_G(U)}$$

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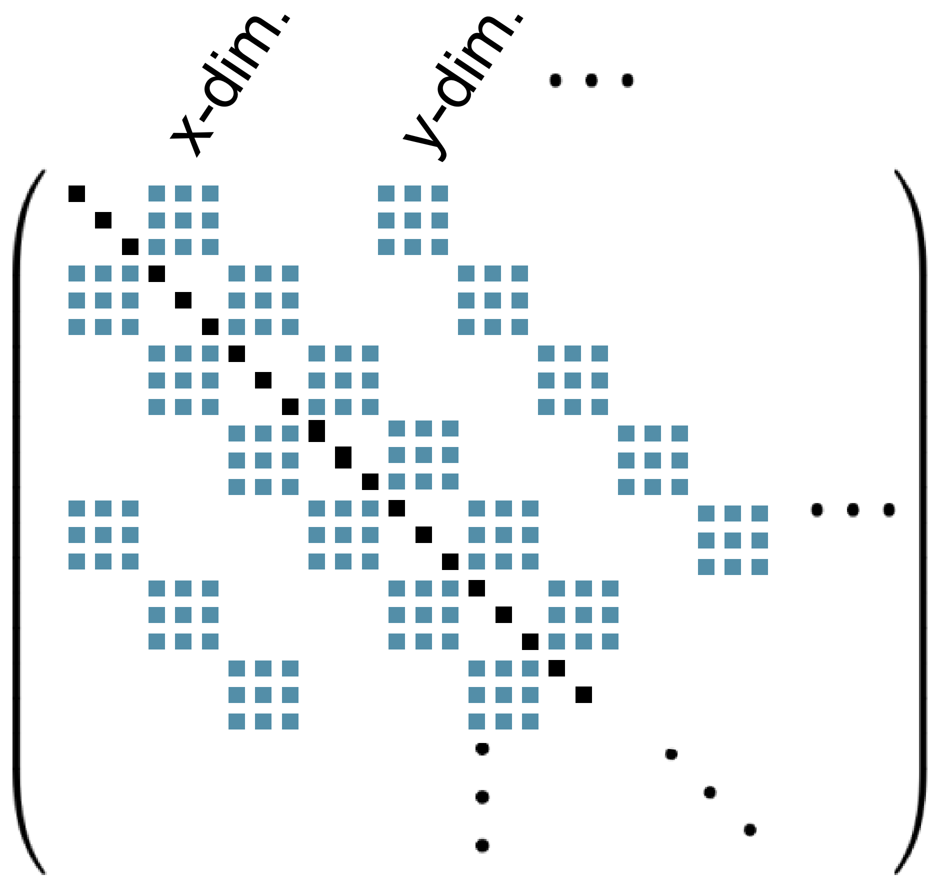


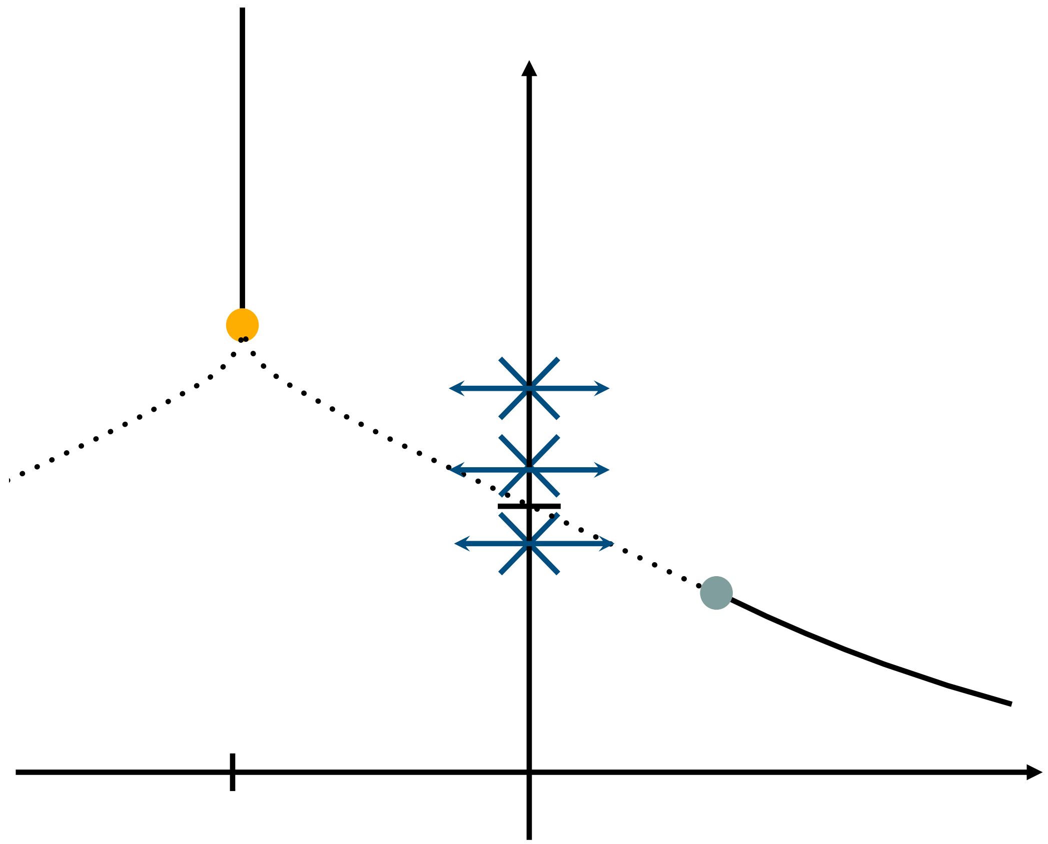
Fermion Determinant:

- Complex at
- Standard MCMC methods become inefficient
- Use Taylor expansion about and simulations at

Fermion matrix: large sparse, band structure is induced by the discretisation of the kinetic terms (derivative), the discretisation is improved by smearing and next-to-next-to nearest interactions

- Calculate derivatives of the pressure

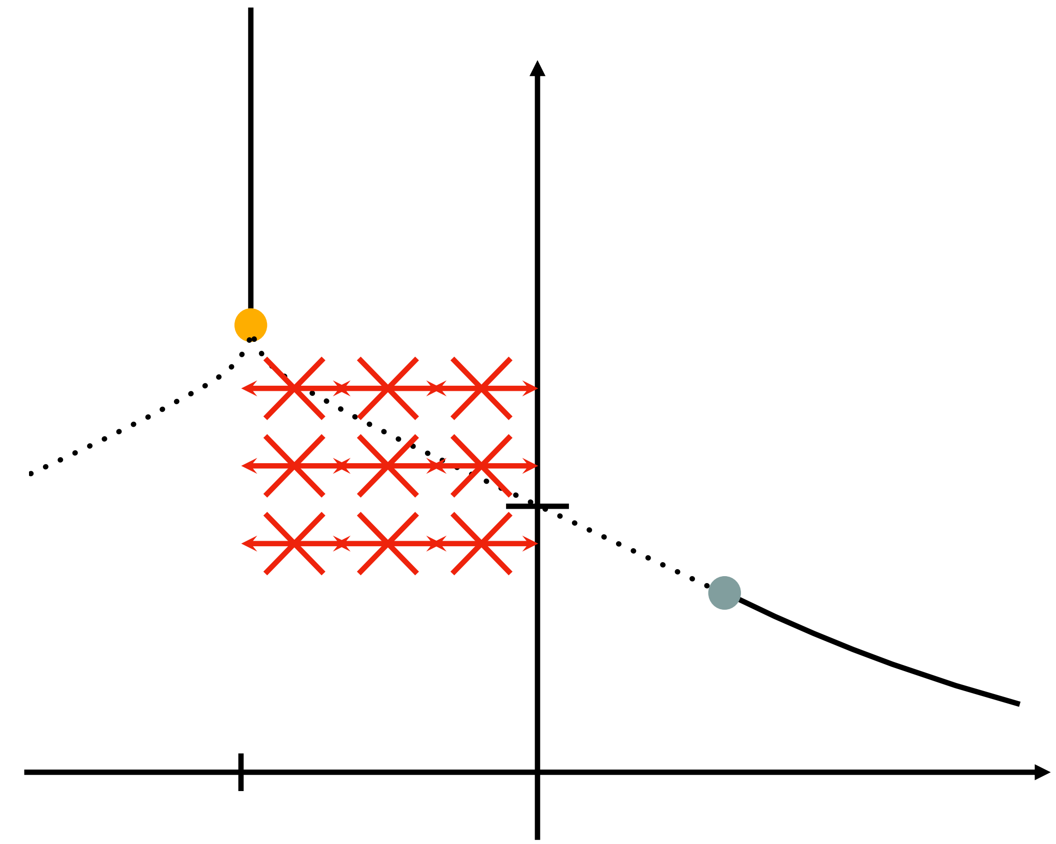
Taylor expansion in



[Allton et al. PRD 66 (2002)]

perform a Padé resummation to obtain the complex singularity that limit the radius of convergence

Taylor expansion in



[De Frorcrand, Philipsen (2002); D'Elia, Lombardo (2003)]

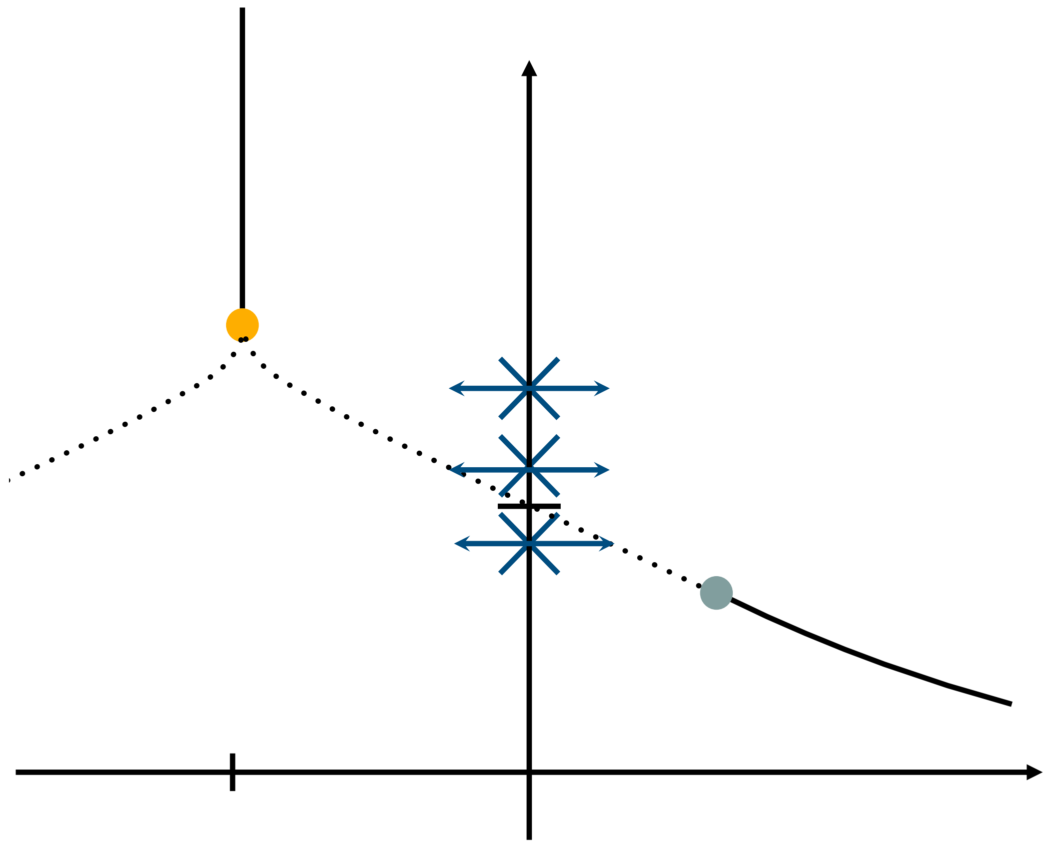
obtain a rational approximation of the data (e.g. by the multi-point Padé) to obtain the closest singularity

alternatively, analyse the (asymptotic) behaviour of the Fourier coefficients

Simulation strategie

- Calculate derivatives of the pressure

Taylor expansion in



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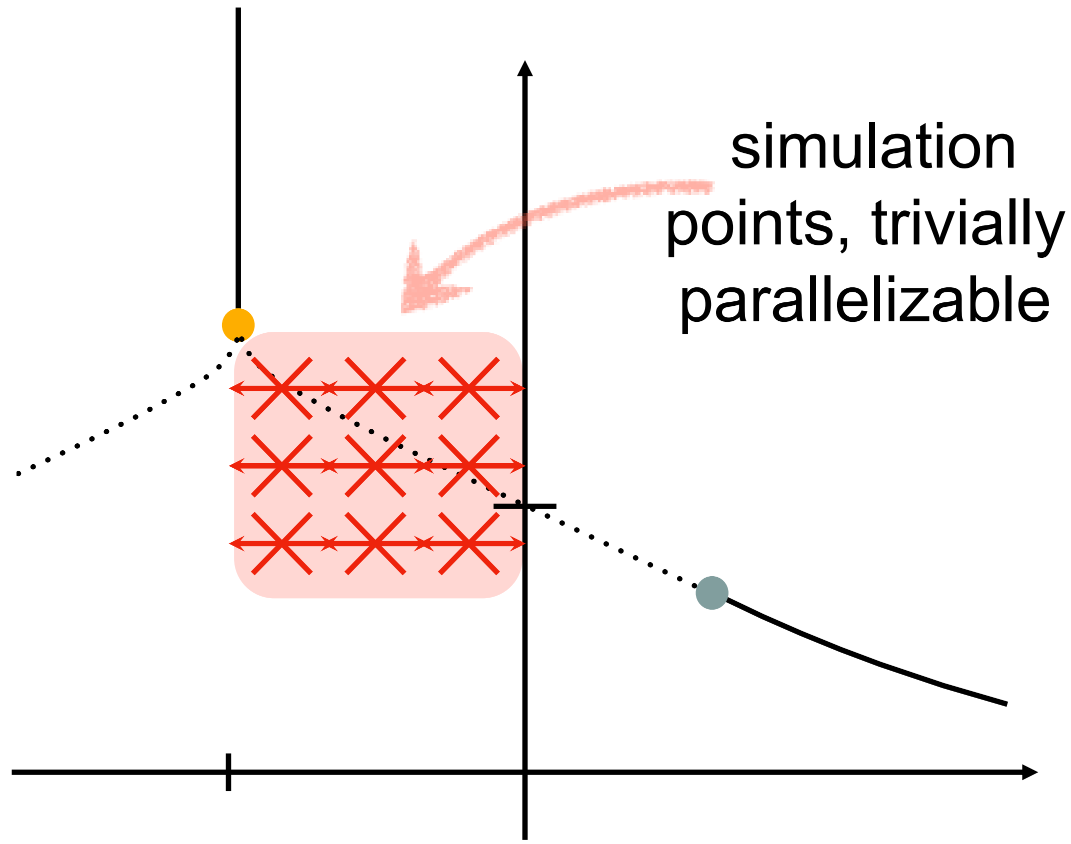

[De Frorcrand, Philipsen (2002); D'Elia, Lombardo (2003)]

obtain a rational approximation of the data (e.g. by the multi-point Padé) to obtain the closest singularity

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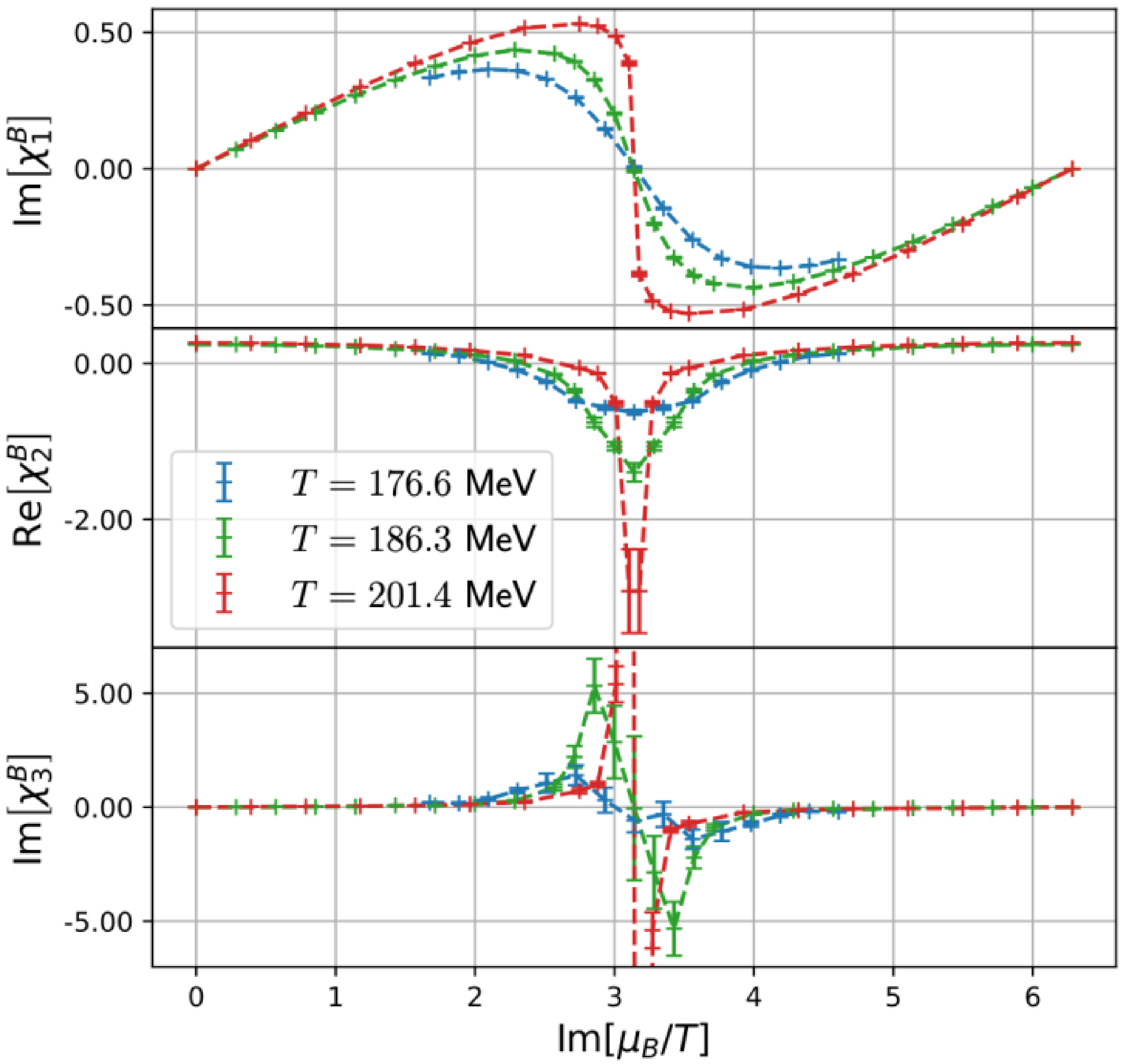
Preliminary results I

Primary simulation output:
cumulants of the baryon number

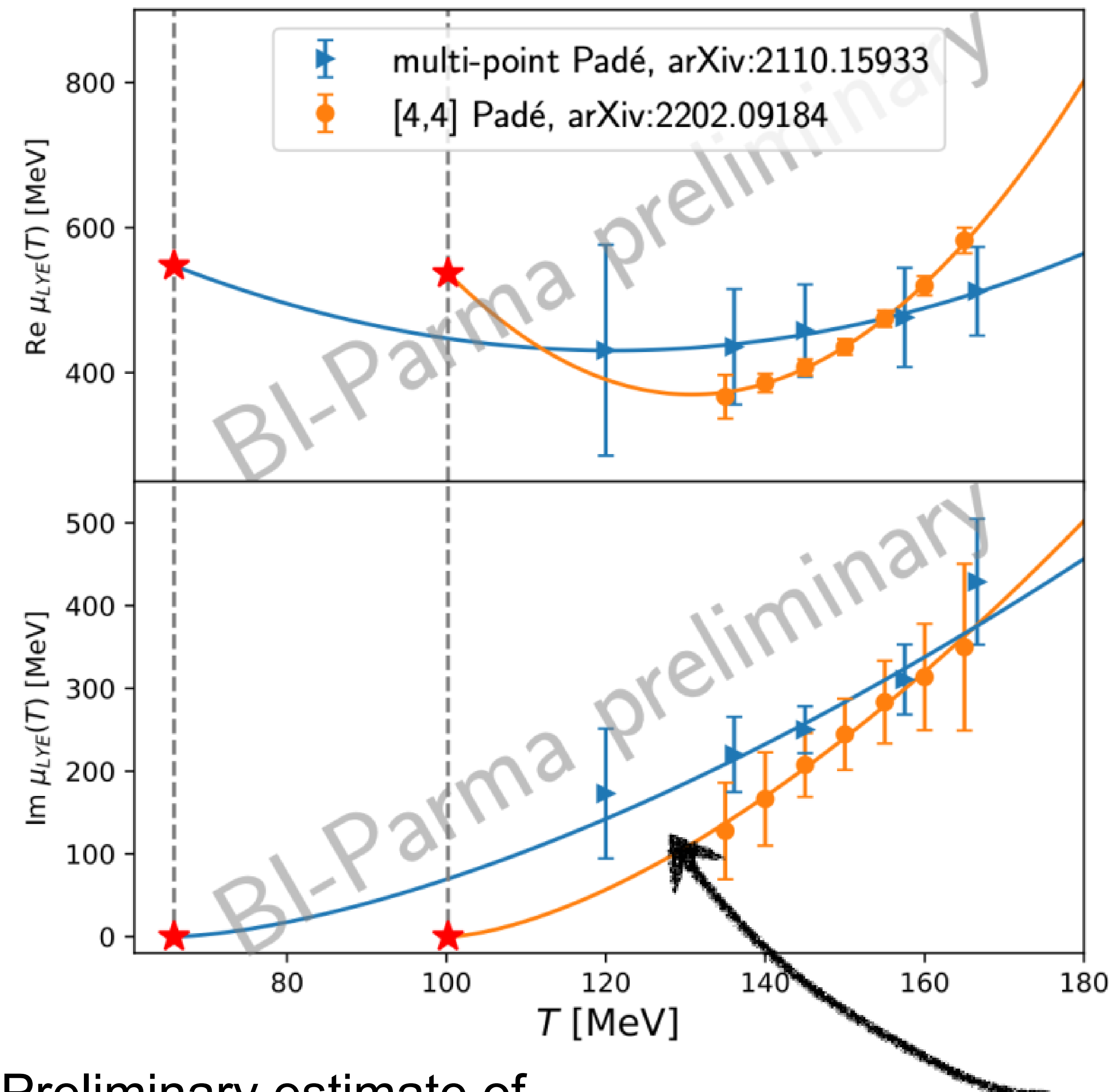


[Dimopoulos et al., *PRD* 105 (2022)]

Analysis steps:

- Perform Padé or multi-point Padé to obtain a rational approximation of the data
- Analyse poles of the rational approximation
- Identify closest pole with the Lee-Yang edge singularity

Preliminary results II



Preliminary estimate of the critical point

Data is consistent with universal scaling

Analysis steps:

- Perform Padé or multi-point Padé to obtain a rational approximation of the data
- Analyse poles of the rational approximation
- Identify closest pole with the Lee-Yang edge singularity
- Tack the singularity as function of temperature
- Extrapolate to the critical point using universal scaling behaviour

SIMULATeQCD

Multi-GPU code developed by our group

- Modern C++ code, uses C++17 features
- Memory management class
- Uses peer-to-peer for inter-node communication
- Uses MPI for communication between notes
- Gauge field generation by Rational Hybrid Monte Carlo
- Multi-shift and multi-RHS conjugate gradient inverter for HISQ fermion matrix
- Code available on GitHub: https://github.com/LatticeQCD/SIMULATeQCD

[Mazur et al, [HotQCD Collaboration] arXiv:2306.01098]

The code is used on various HPC systems

- Piz Daint@CSCS: 21 PFlop/s
- Juwels-Booster@JSC: 44 PFlop/s
- Summit@ORNL: 122 PFlop/s
- Leonardo@CINECA: 238 PFlop/s
- LUMI@CSC: 379 PFlop/s

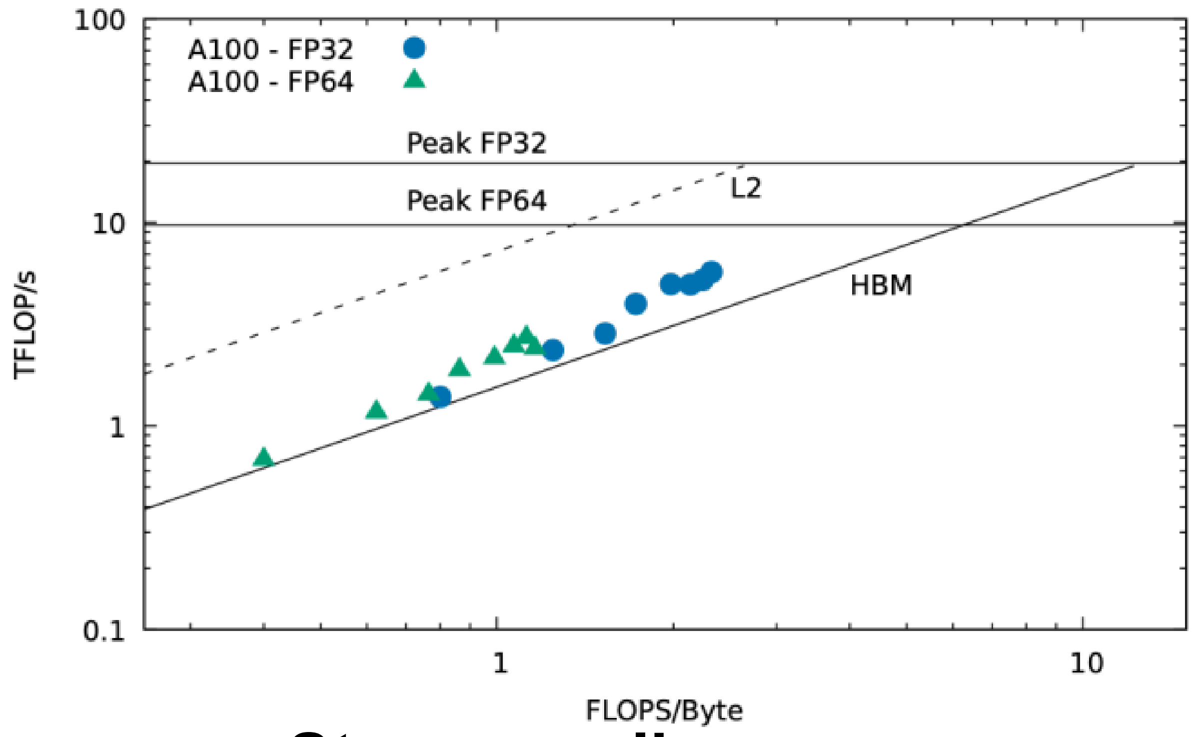
GPUs: Nvidia, AMD

Summit

Leonardo

LUMI

- Spend most of the time in the Matrix*Vector application
- Arithmetic intensities are low: 0.73 (FP32), 0.36 (FP64)
- Increase Intensities by introducing multiple () RHS

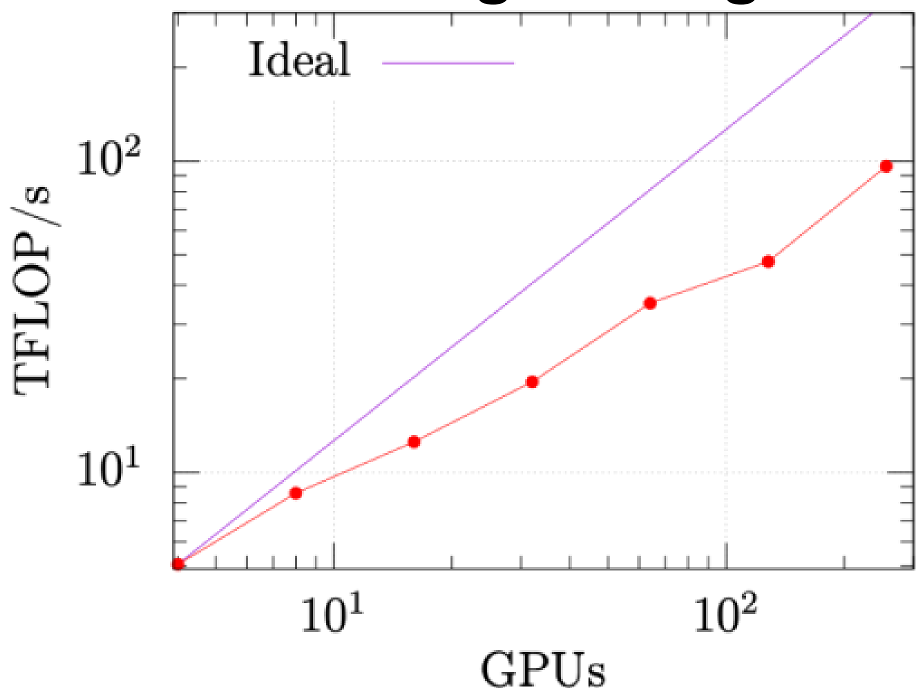


Roofline model

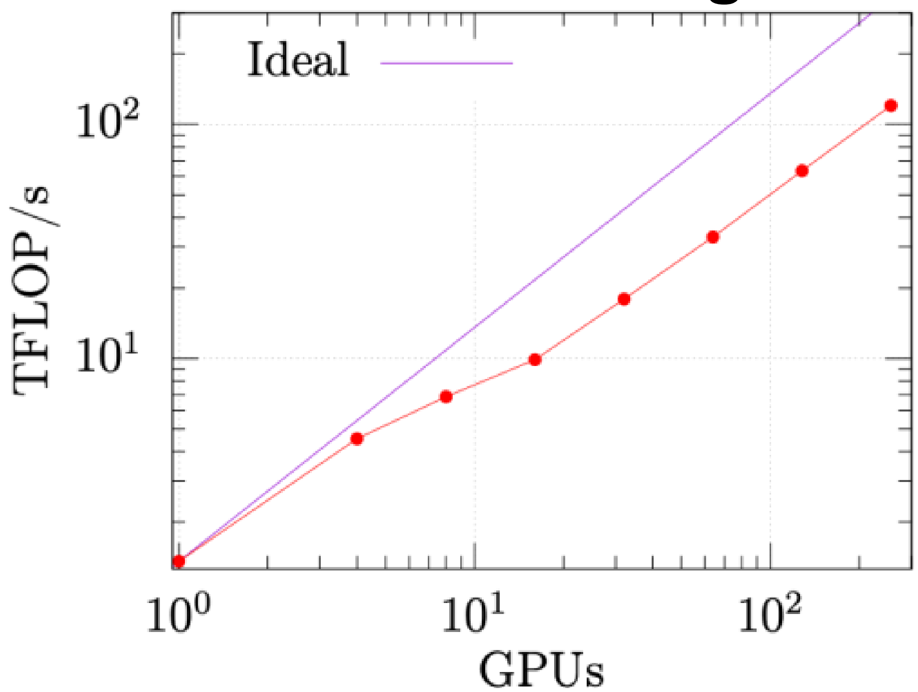
2.81 (FP32)

[Mazur et al, [HotQCD Collaboration] arXiv:2306.01098]

Strong scaling



Weak scaling



- Current efforts in optimisation of SIMULATeQCD on LUMI-G/AMD GPUs are supported by the EuroHPC extraordinary support program (ESP).

New physics in the muon magnetic moment?

EUROHPC USER DAY 2023 Brussels 11.12.23

Project: "EHPC-EXT-2023E02-063"

EuroHPC used: Leonardo Booster

Speaker: Bálint TÓTH (University of Wuppertal)

Acknowledgements

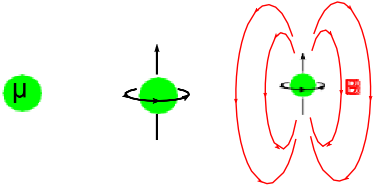
- Budapest-Marseille-Wuppertal (BMW) Collaboration

  Sz. Borsányi, Z. Fodor, J. N. Günther, C. Hoelbling, S. D. Katz, L. Lellouch, T. Lippert, K. Miura, L. Parato, K. K. Szabó, F. Stokes, B. C. Tóth, Cs. Török, L. Varnhorst

- Nature 593 (2021) 7857, 51-55 [arXiv:2002.12347]
- We acknowledge PRACE for awarding this project access to HAWK hosted by the High-Performance Computing Center Stuttgart.
- The computer time for this work were provided in part by the Gauss Centre for Supercomputing on the machines JUWELS, SUPERMUC and HAWK.

The muon

- Elementary particle
- Created by cosmic rays entering the atmosphere
- ≈ 207 times heavier than electron, same charge and spin
- Acts like a tiny magnet



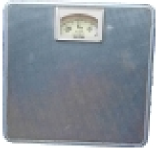
How strong is its magnetic moment? $g_\mu = ?$

- Can be measured experimentally
- Can be computed from the Standard Model (SM)
- If theory disagrees with experiment $\longrightarrow$ New physics?

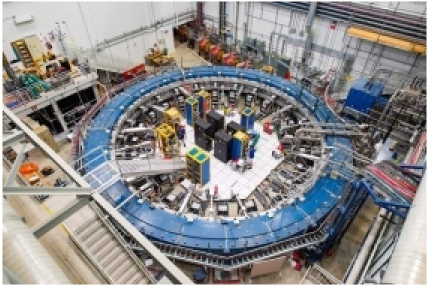
Experiment

- Brookhaven 2004: $a_\mu^{\text{BNL}} = 11659209.1(6.3) \times 10^{-10}$
- Fermilab 2023: $a_\mu^{\text{FNAL}} = 11659205.5(2.4) \times 10^{-10}$
- Combined: $a_\mu^{\text{exp.}} = 11659205.9(2.2) \times 10^{-10}$

Precision: bathroom scale sensitive to weight of a single eyelash.



- $a_\mu = \frac{g_\mu - 2}{2}$

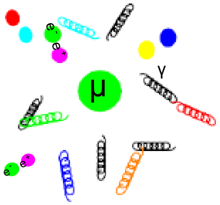


Muon storage ring at Fermilab

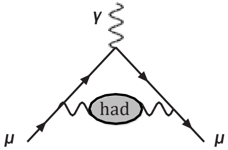
Theory: Standard Model (SM)

Sum over all known physics:

1. quantum electrodynamics (QED): photons, leptons
2. electroweak (EW): W, Z bosons, neutrinos, Higgs
3. strong (QCD): quarks and gluons



Hadronic vacuum polarization (HVP) of photon:

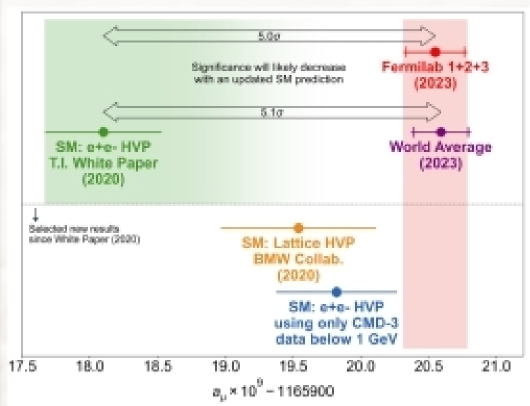
$a_\mu^{\text{LO-HVP}} =$ 

dominates theory uncertainty

Two methods:

- e+e- HVP
  Needs $e^+ e^- \to$ hadrons cross section data
- Lattice HVP
  Ab initio method ←− this work

Current status

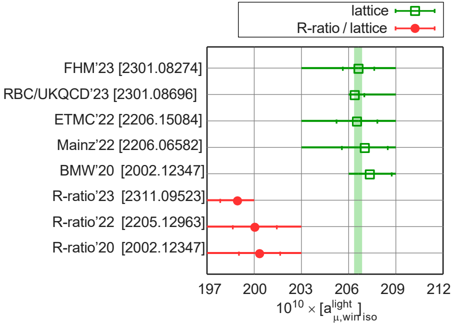


[Plot from Run2/3 announcement on 10th Aug 2023 at Fermilab]

- e+e- HVP
  Differs by more than 5σ from Fermilab.
- e+e- HVP using CMD3 data
  - Removes discrepancy with Fermilab.
  - Not yet scrutinized by e+e- HVP community.
- Lattice HVP
  First full computation was done by our group.
  No strong tension with Fermilab, only 1.7σ.

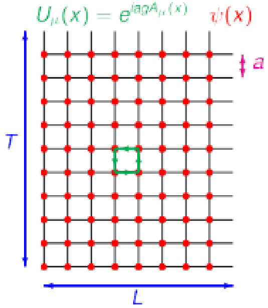
HVP-window

- Part of HVP: Restrict correlator to window between $t_1 = 0.4\,\text{fm}$ and $t_2 = 1.0\,\text{fm}$ [RBC/UKQCD'18]
- Easily computable on lattice
- Can be computed from e+e- HVP as well
- Latest result from each group $\longrightarrow$ consensus within lattice community
- Significant discrepancy between e+e- HVP and lattice



Lattice QCD

- Lattice gauge theory: systematically improvable, non-perturbative, 1st principles method
- Discretize space-time with lattice spacing: a



- quarks on sites, gluons on links
- discretize action + operators

$$\int \mathrm{d}^4x \longrightarrow a^4 \sum_x$$

$$\partial_\mu \longrightarrow \text{finite differences}$$

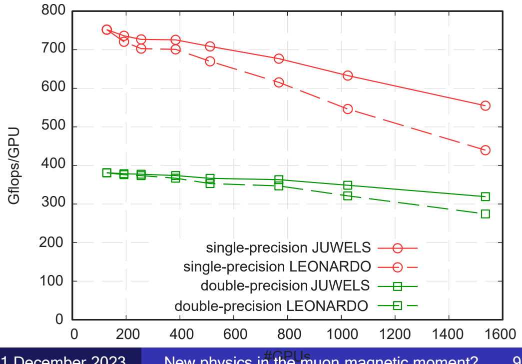
- To get physical results, need to perform:
  1. Infinite volume limit $(V \to \infty)$
  2. Continuum limit $(a \to 0)$

Lattice QCD

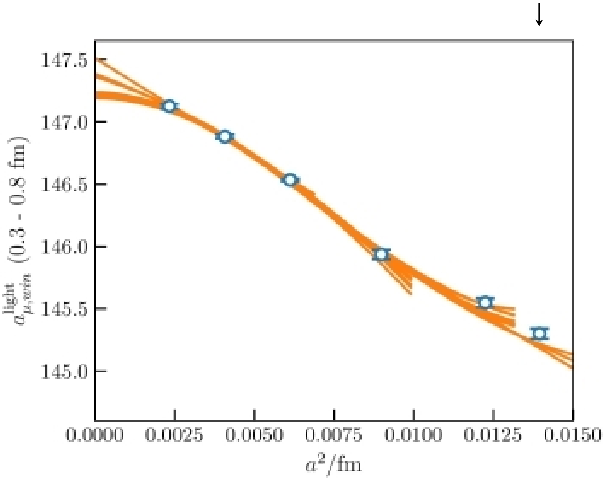
- Integrate over all classical field configurations

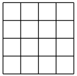
$$\int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\; O\; e^{-S_g(U)-\overline{\psi}M(U)\psi}$$

- E.g. $176^3 \times 264$ lattice $\longrightarrow \approx 5 \cdot 10^{10}$ dimensional integral
- Stochastic integration



Continuum limit





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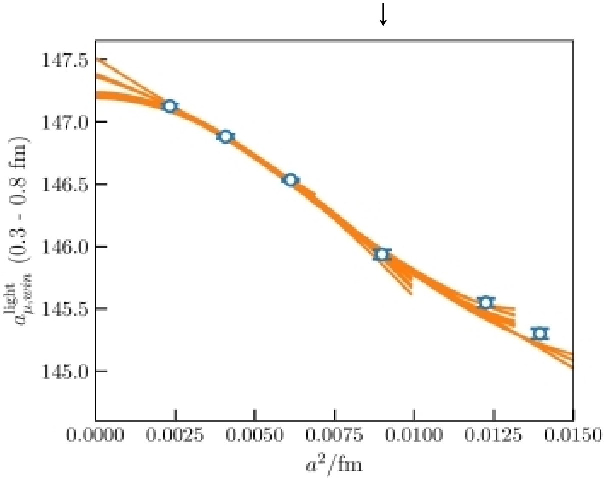

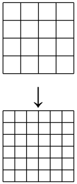

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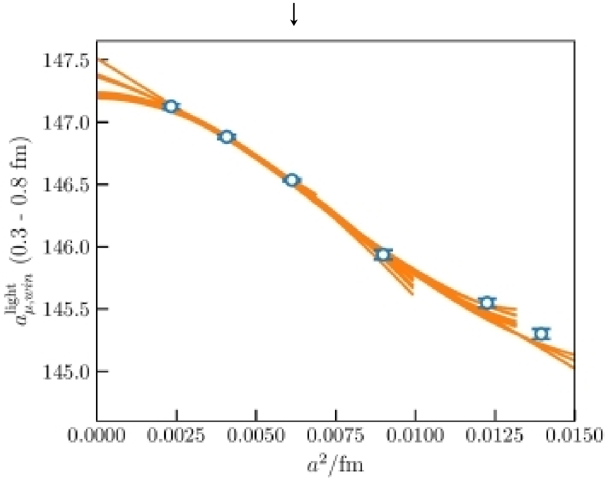

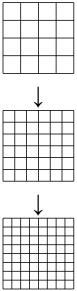

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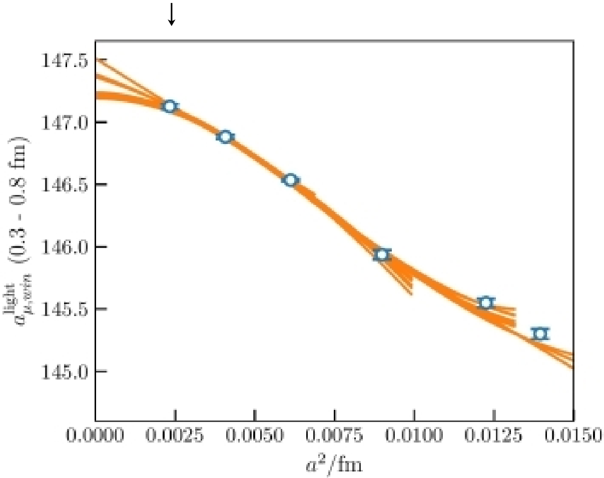

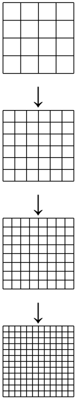

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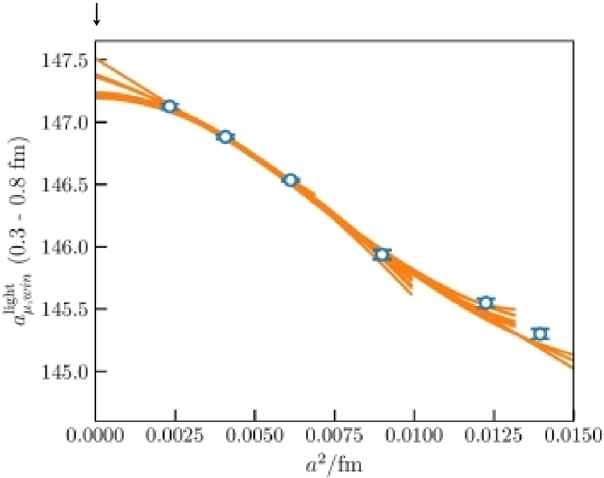
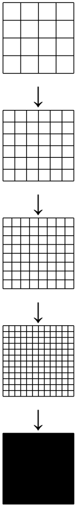
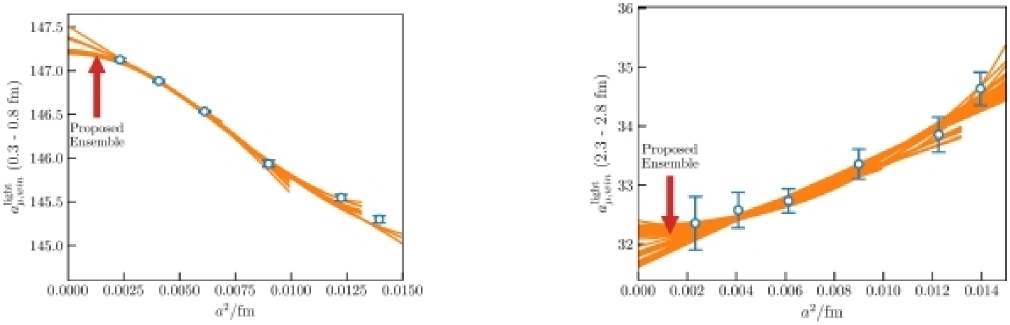




Finer/larger lattices



- Largest source of systematic uncertainty: continuum extrapolation
- Proposed ensemble at $a = 0.036\,\text{fm}$, $176^3 \times 264$ can further constrain fits

Summary & Outlook

- HVP-window:
  - Agreement among different lattice groups
  - Disagreement between e+e- HVP and lattice

  $\longrightarrow$ Has to be understood before New Physics can be announced or ruled out

- Experiment:
  - Important to pursue $e^+ e^- \to \text{hadrons}$ experiments
  - MUonE experiment will provide data relevant for further cross-checks

- Lattice:
  - To keep up with future precision of Fermilab experiment factor 4x reduction of uncertainty on HVP is needed
  - Improve continuum extrapolation $\longleftarrow$ finer lattice

What do spin glasses have to say about quantum optimization?

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

Project: “*Quantum spin glasses on the GPU*”

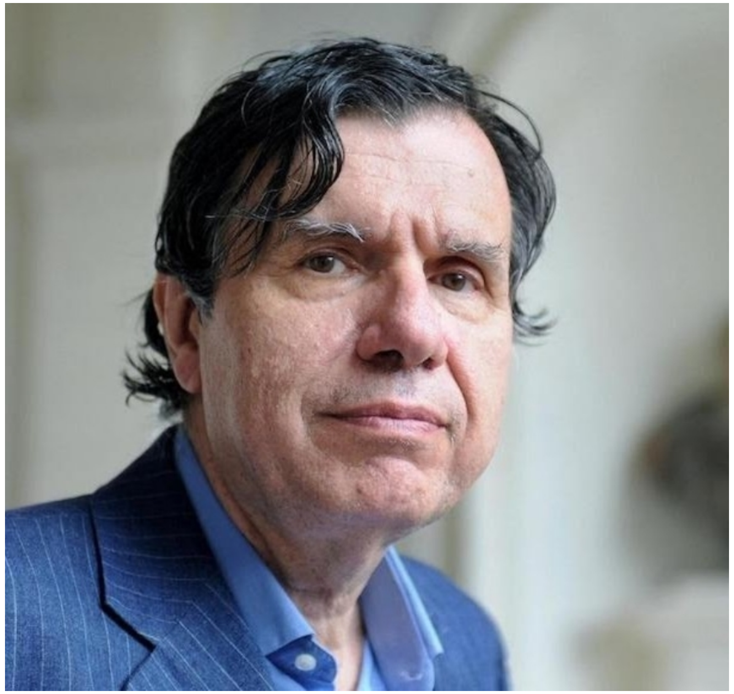
EuroHPC used: MeluXina and Leonardo (LEAP)

Collaborators

arXiv:2310.07486

Massimo Bernaschi

Víctor Martín Mayor



Giorgio Parisi

Computational problems

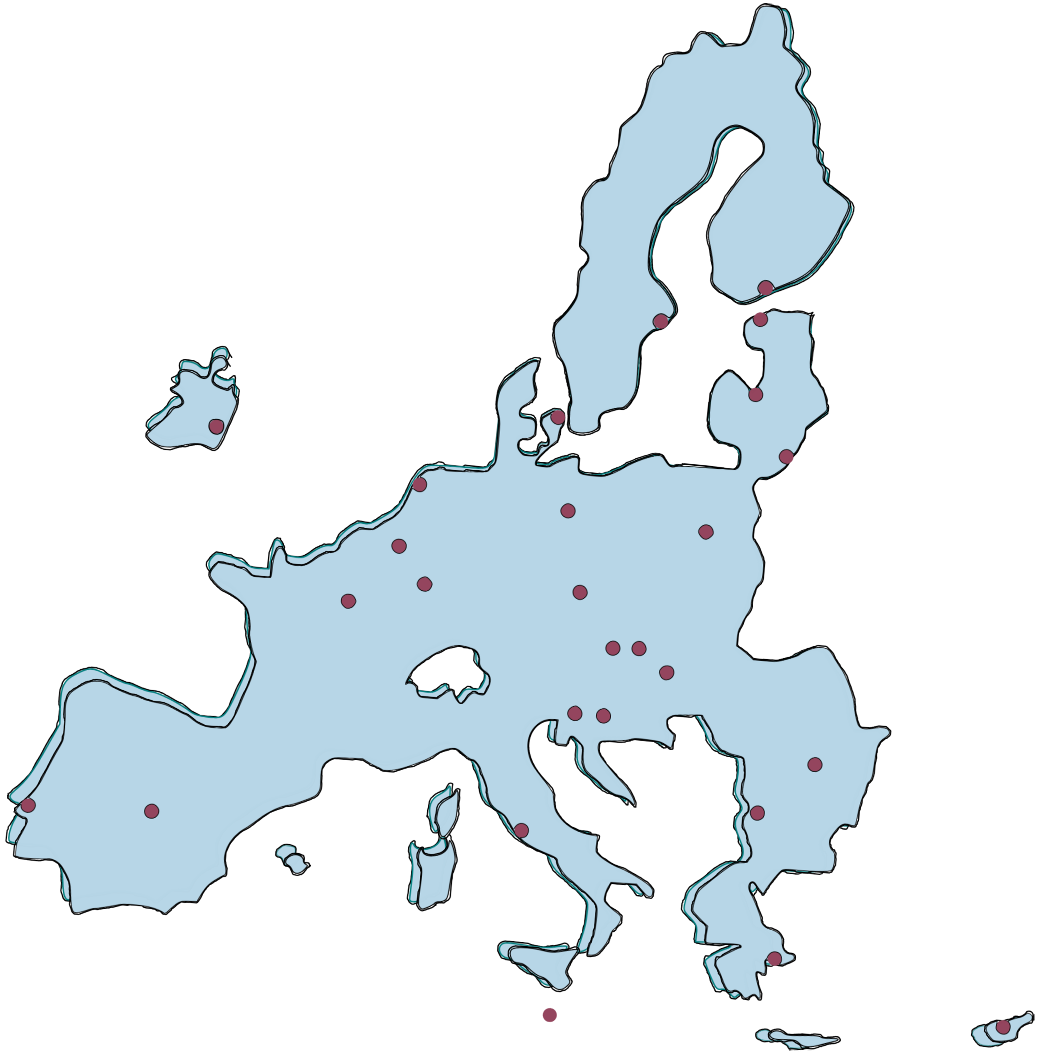
- Let us consider **N** cities:
  - **Easy** problem: sort by name

    CPU time scales as $N \log N$

  - **Hard** problems: organize a train trip along them

    Minimize cost, path length…

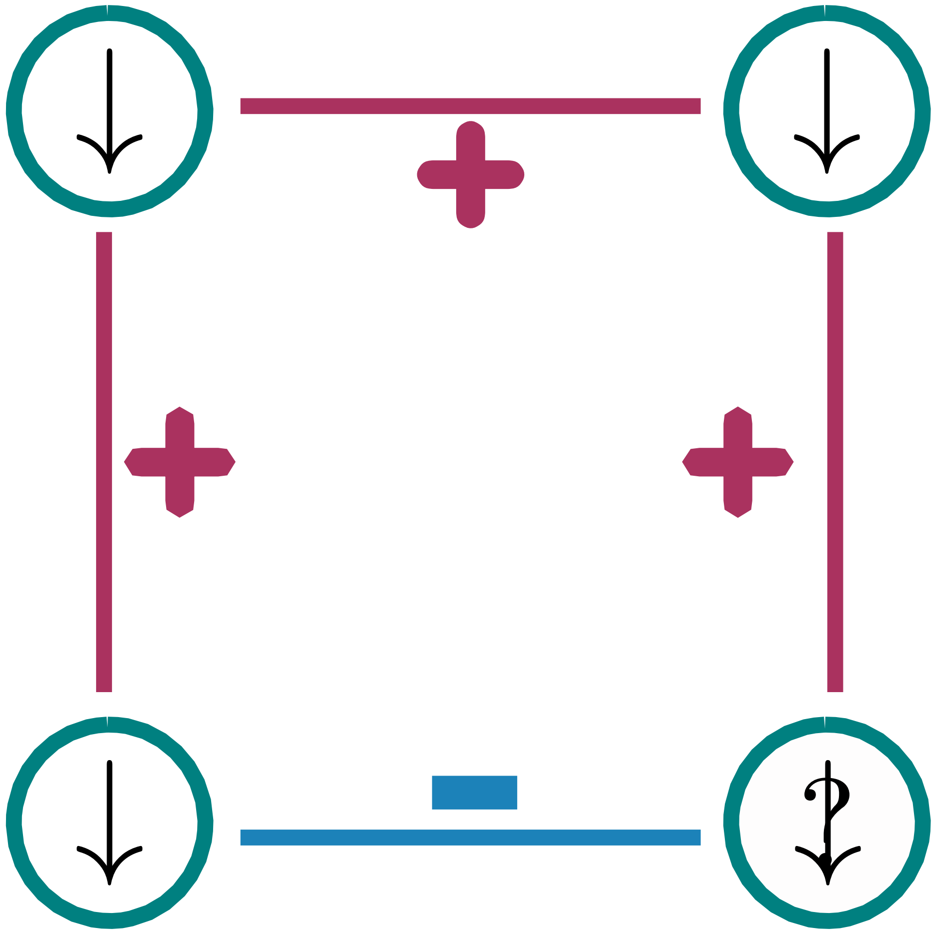
  - **NP** problem



Spin glasses: a NP problem

- Energy:

$$H = -\sum_{\langle i,j \rangle} J_{ij} s_i s_j$$



Spin glasses: a NP-complete problem

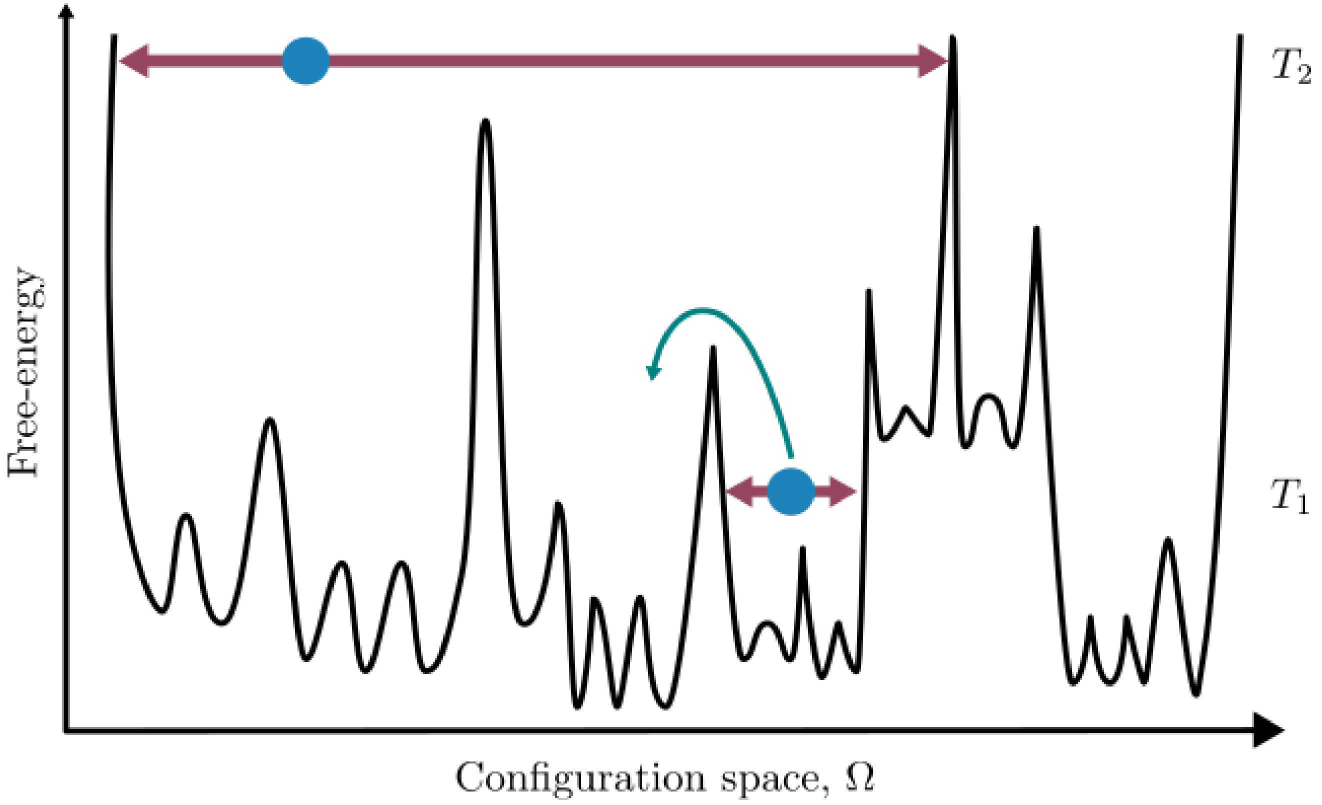
- Energy:

$$H = -\sum_{\langle i,j \rangle} J_{ij} s_i s_j$$

- Minimize the energy

⬇

NP-complete



Quantum Computing

“Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical.”

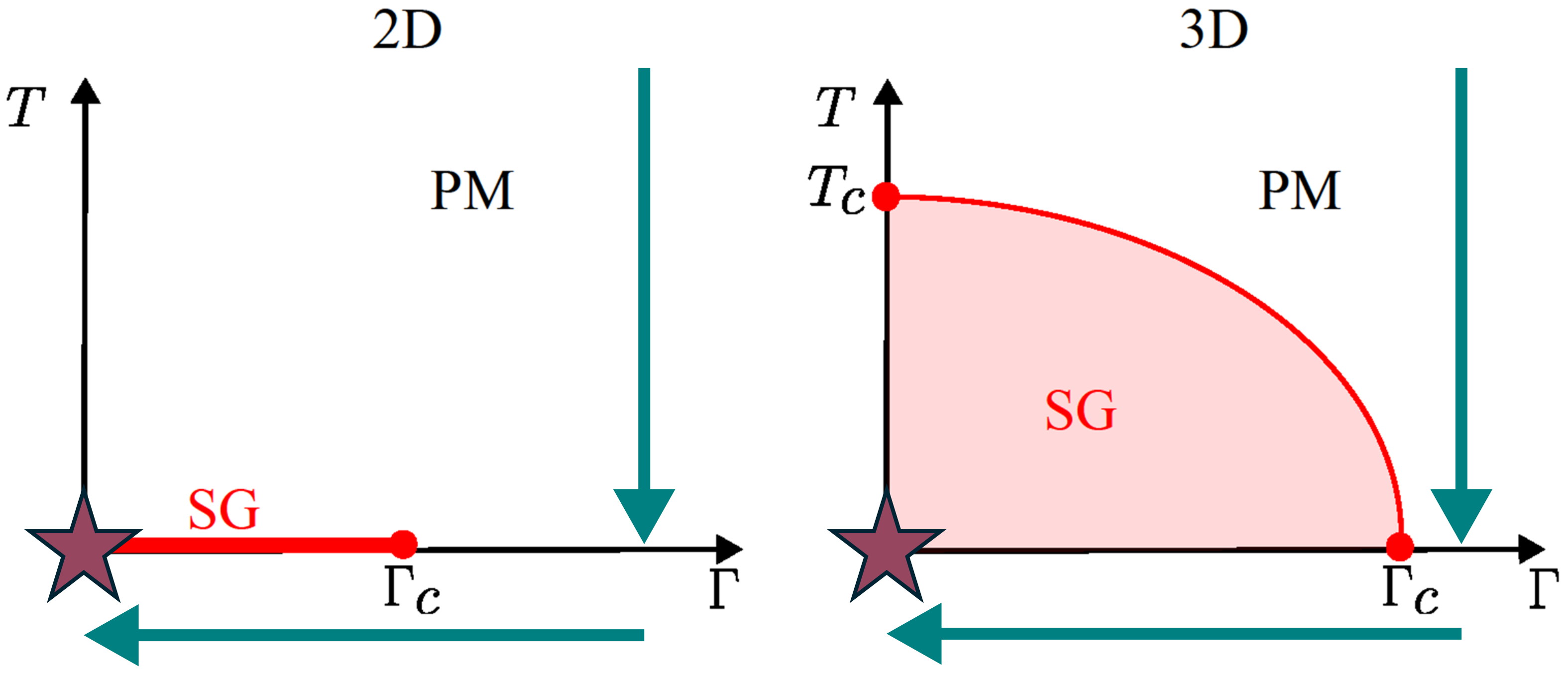
R. Feynman

Quantum spin glasses

$$\hat{H} = -\sum_{\langle i,j \rangle} J_{ij} \hat{\sigma}_i^Z - \Gamma \sum_i \hat{\sigma}_i^X$$

- Reduce Γ
- **Adiabatically**

$$t_{\text{an}} \propto \frac{1}{\Delta E^2} = L^{2z}$$



Extensive GPU simulations

We studied D = 2

- Trotter-Suzuki approximation

$\hat{H}$ in **D**-dimensions → H in (**D** +1)-dimensions

Quantum | Classic

$$Z = \mathrm{Tr}\,\hat{T}$$

$$Z = \mathrm{Tr}\,T$$

$$\Gamma = \frac{-1}{2k}\log[\tanh\ k]$$

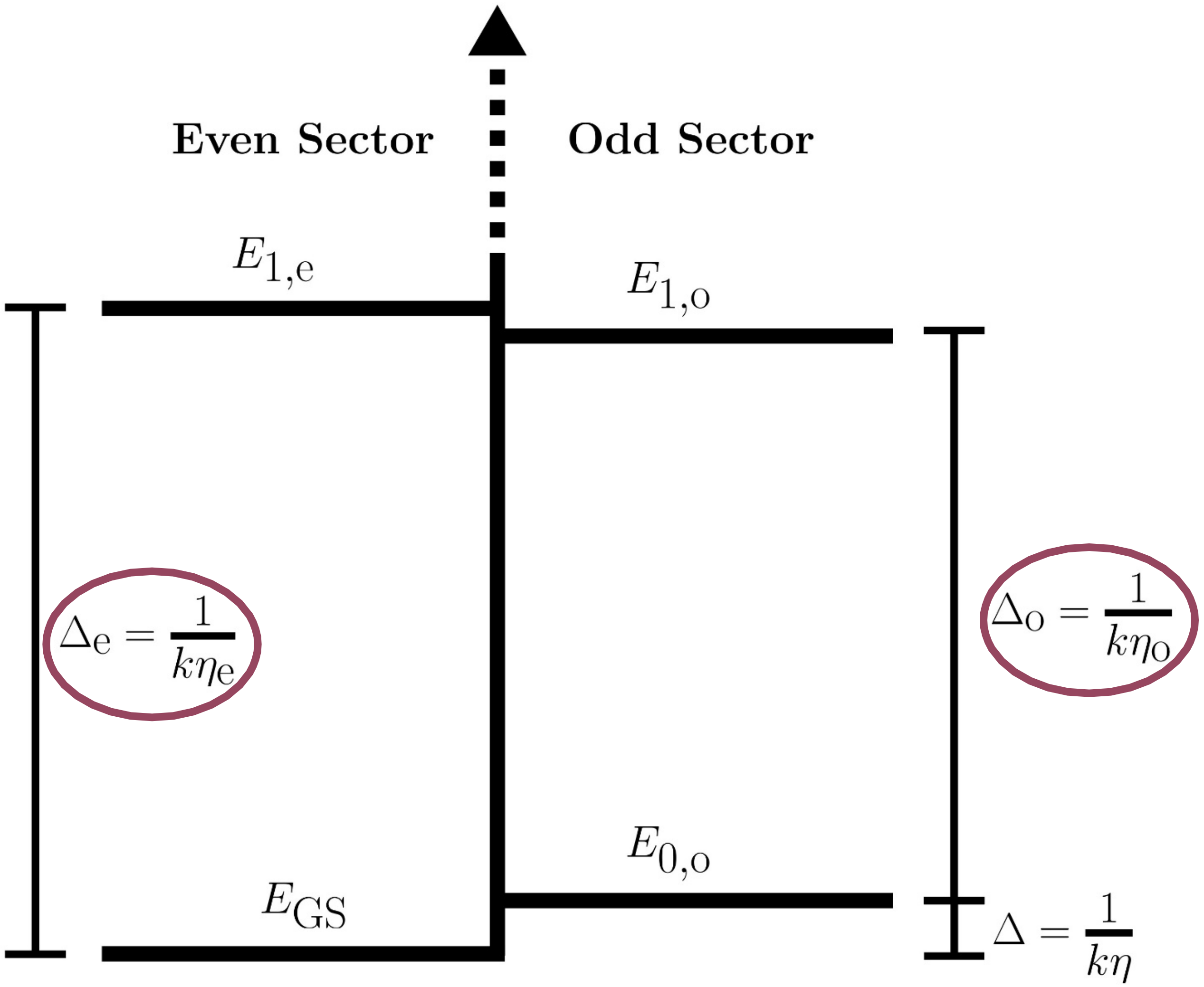
k grows → Γ decreases

Extensive GPU simulations

- Parity symmetry ($\hat{P}$)

$$\hat{P} = \prod_i \hat{\sigma}_i^X$$

$$\hat{H} = \hat{H}_{\mathrm{e}} \oplus \hat{H}_{\mathrm{o}}$$

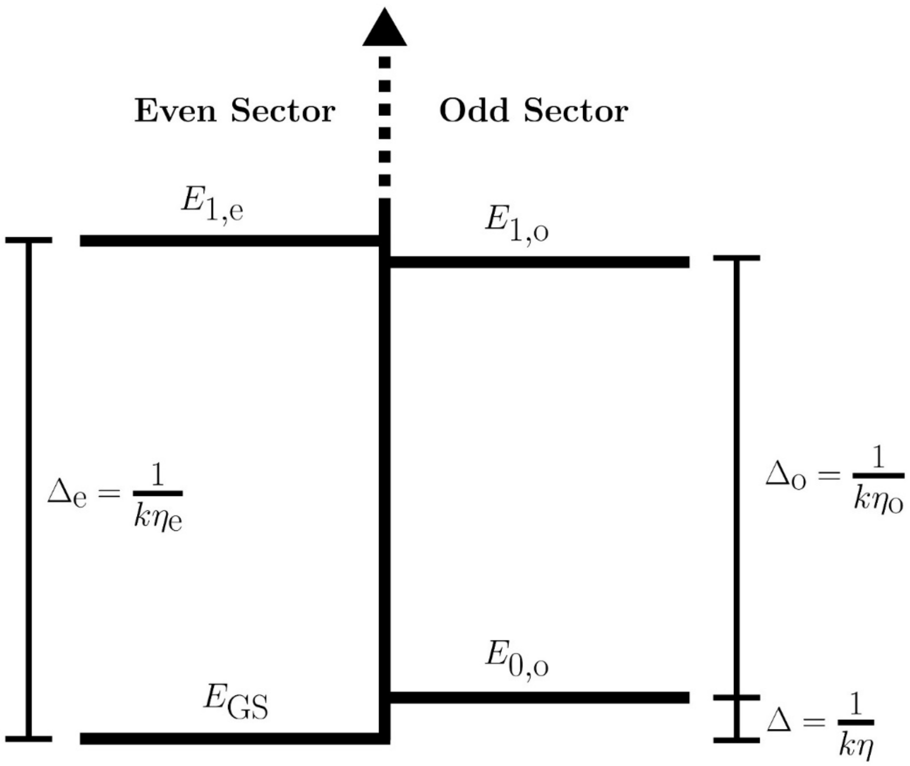


Exact diagonalization

- Diagonalize Transfer Matrix T
- T is a $2^{L\times L} \times 2^{L\times L}$ matrix:
  - $L = 5 \rightarrow 2^{25} \times 2^{25}$
  - $L = 6 \rightarrow 2^{36} \times 2^{36}$
- Using Parity:
  - $L = 6 \rightarrow 2^{35} \times 2^{35}$

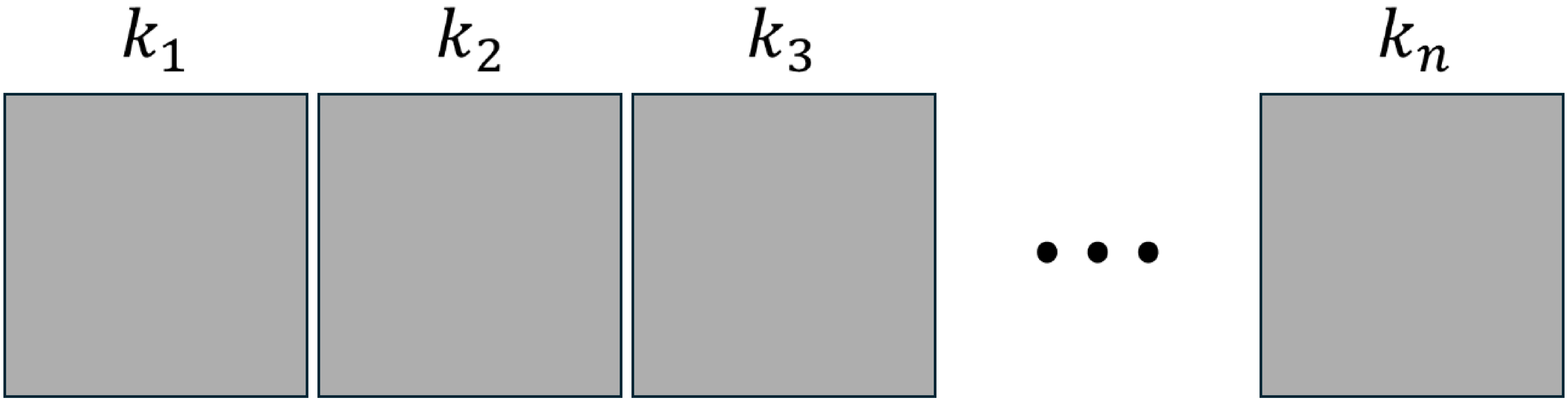
At least **16 GPUS**!

- We used PetSc and Slepc libraries
- (Very) *custom* matrix-vector multi-GPU-CPU product for Lanczos algorithm



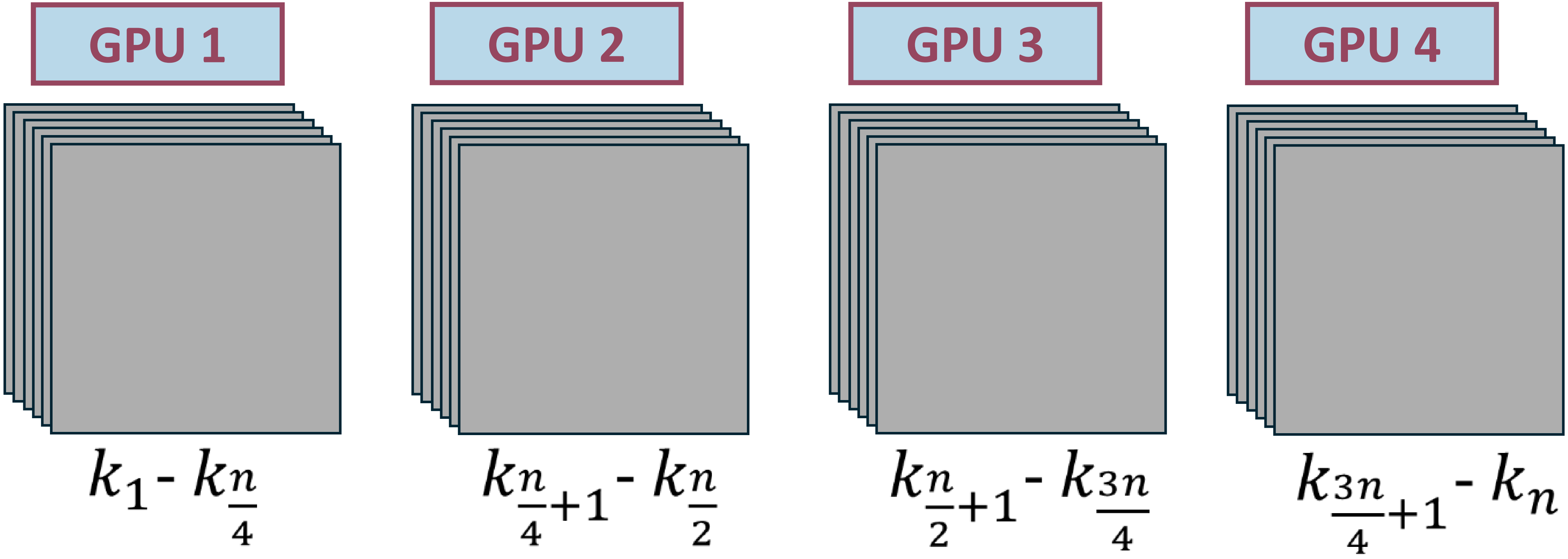
Monte Carlo simulations

- Parallel Tempering: $(k_1, k_2, \cdots, k_n)$



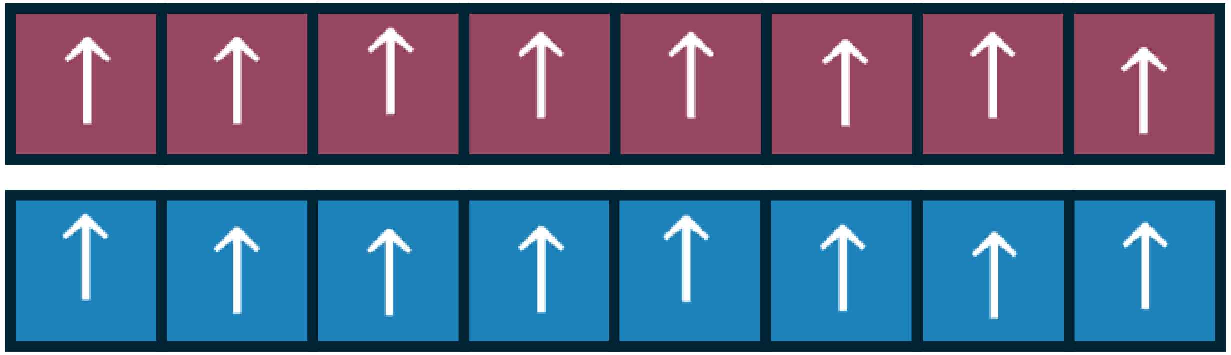
Monte Carlo simulations

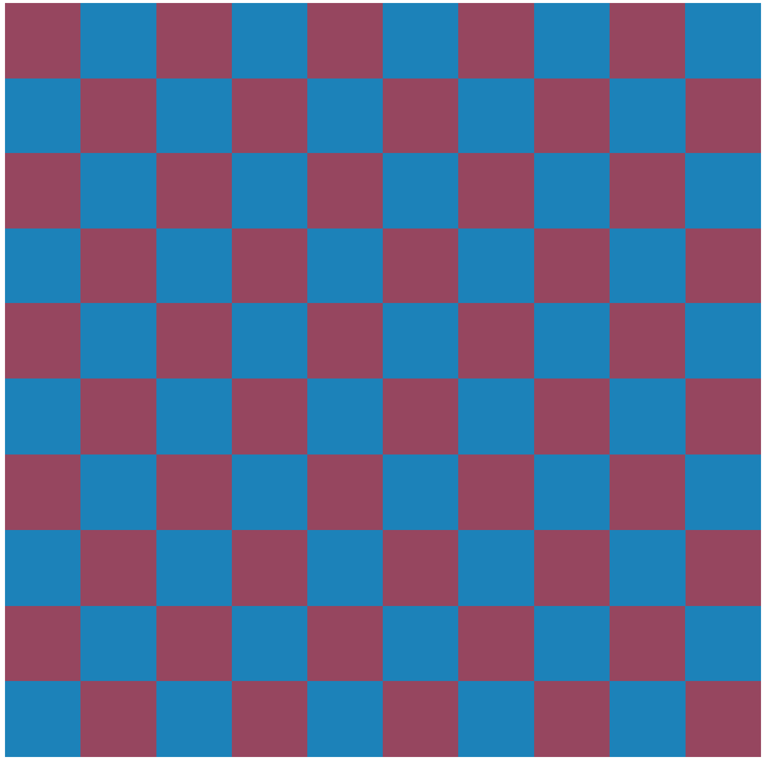
- Parallel Tempering: $(k_1, k_2, \cdots, k_n)$



Monte Carlo simulations

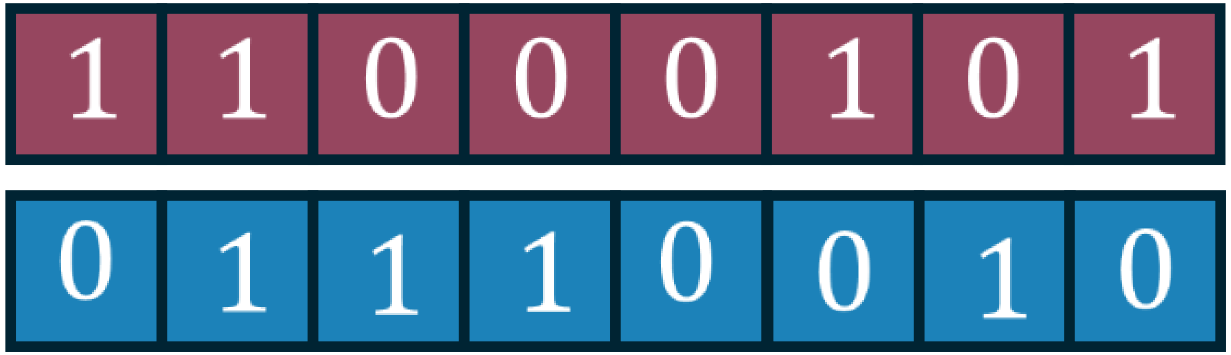
- Parallel Tempering: $(k_1, k_2, \cdots, k_n)$
- Checkerboard decomposition
- MUlti-SIte multispin coding
- **32-bit** words

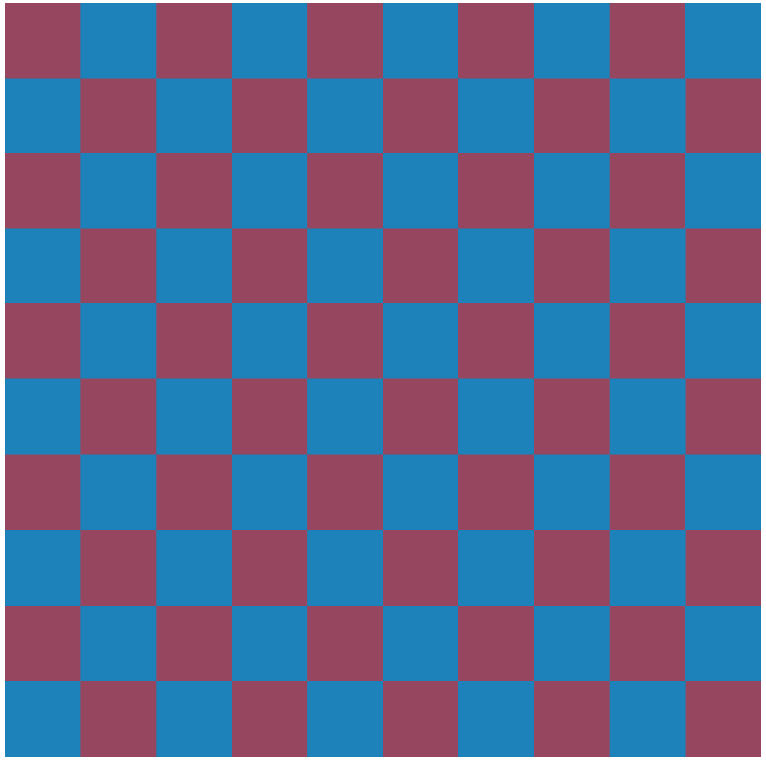




Monte Carlo simulations

- Parallel Tempering: $(k_1, k_2, \cdots, k_n)$
- Checkerboard decomposition
- MUlti-SIte multispin coding
- **32-bit** words





Monte Carlo simulations

- Random bits for MUSI (briefly):
  1. Implement a CUDA version of `philox_4x32_10` **D.E. Shaws**
     - `(x4) 32-bit words "50/50"`
  2. `philox_4x32_10` + `xoroshiro128++` **S. Vigna**
     - (x4) 64 bits "50/50"
  3. Transform 64 "50/50" bits into 8 bits with desired probs.

  ➢ (`philox_4x32_10` + `xoroshiro128++`) → **32-bits**

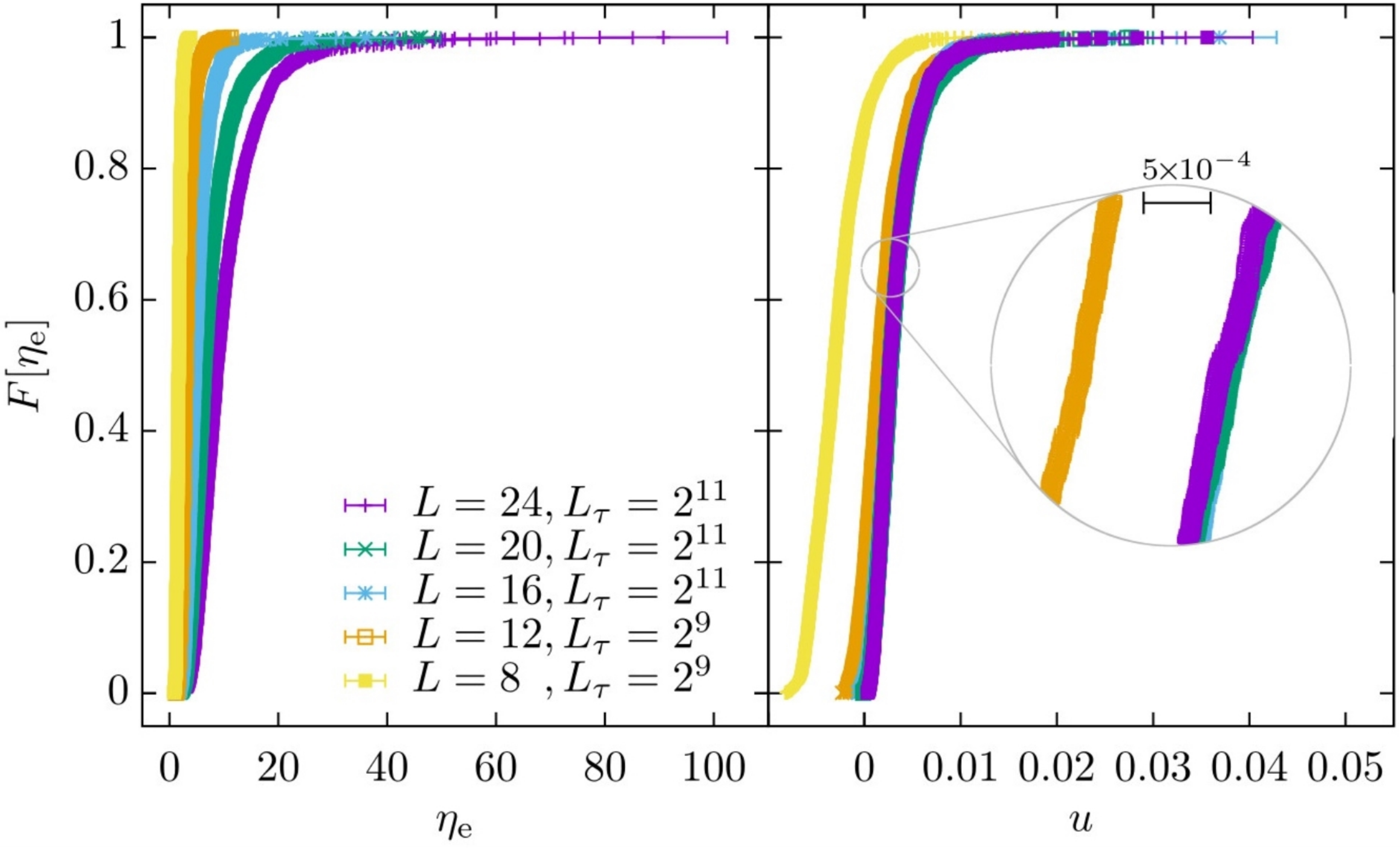
➢ **0.5 ps per spin update!**

➢ **2.5 core-Mhours in Meluxina GPU+ ~3 GPU-Mhours in Leonardo**

Monte Carlo simulations (main result)

$$u = \frac{\eta_e - \eta_e^0}{L^{z_e}}$$

$$\eta_e^0 = 2.2(3)$$
$$z_e = 2.46(17)$$



Conclusions

arXiv:2310.07486

- We studied Quantum Phase Transition in **D=2:**

$$k_c = 0.2905(5), \qquad \frac{1}{\upsilon} = 0.70(24)(9),$$

$$\frac{\gamma^{(2)}}{\upsilon} = 0.27(8)(8), \qquad \frac{\gamma^{(3)}}{\upsilon} = 1.39(23)(11)$$

- **Parity** symmetry splits the configuration space.
- There are two dynamic exponents:

$$\mathbf{z_e = 2.46(17)}, \qquad z \sim \infty$$

What do spin glasses have to say about quantum optimization?

There are no theoretical restrictions when crossing the Quantum Phase Transition in Quantum Annealing

Project: *“Quantum spin glasses on the GPU”*

EuroHPC used: MeluXina and Leonardo (LEAP)

What next?

- Focus on hard problems (samples).
- Simulate only the even sector.
- Add second-neighbor interaction.
- What happens at D=3?
- Go from Γ_c to $\Gamma = 0$.

Multi-scale microstructure modeling for corrosion and hydrogen embrittlement

EUROHPC USER DAY 2023 Brussels 11.12.23

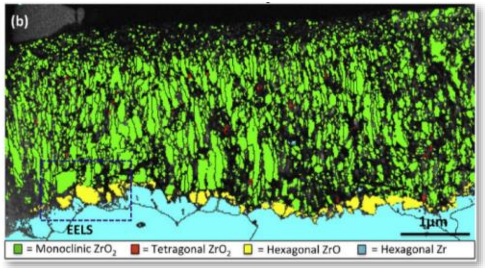
Project: *Microstructure modeling*

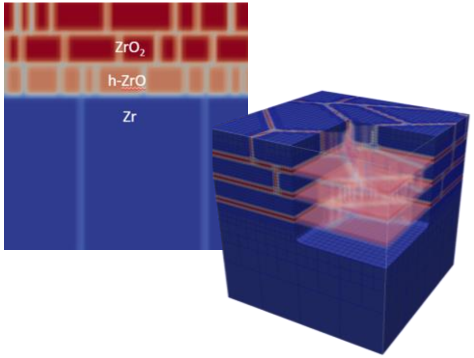
EuroHPC used: LUMI-C

Speaker: Alexander Mavromaras, Materials Design

Executive Summary

- **Industry Challenges:** Corrosion and hydrogen embrittlement pose significant challenges across numerous industries
- **Mitigation Strategies** necessitate a comprehensive understanding and control of the material's microstructure
- **The Value of Simulations:** Multi-scale simulations insights and data where experiments are costly and time-consuming
- **Collaborative Approach:** Materials Design is developing a multi-scale modeling approach together with industrial and academic partners.
- **Case Study:** The evolution of microstructure during the oxidation of metals, such as zirconium alloys





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Overview

- **Company Snapshot**

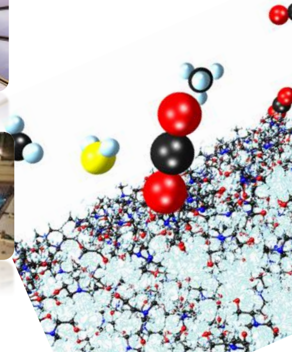
  Materials Design - A Brief Overview of the Company and Its Technology.
- **Material Challenges**

  Exploring Corrosion and Hydride Formation in Zirconium Alloys.
- **Bridging the Gap**

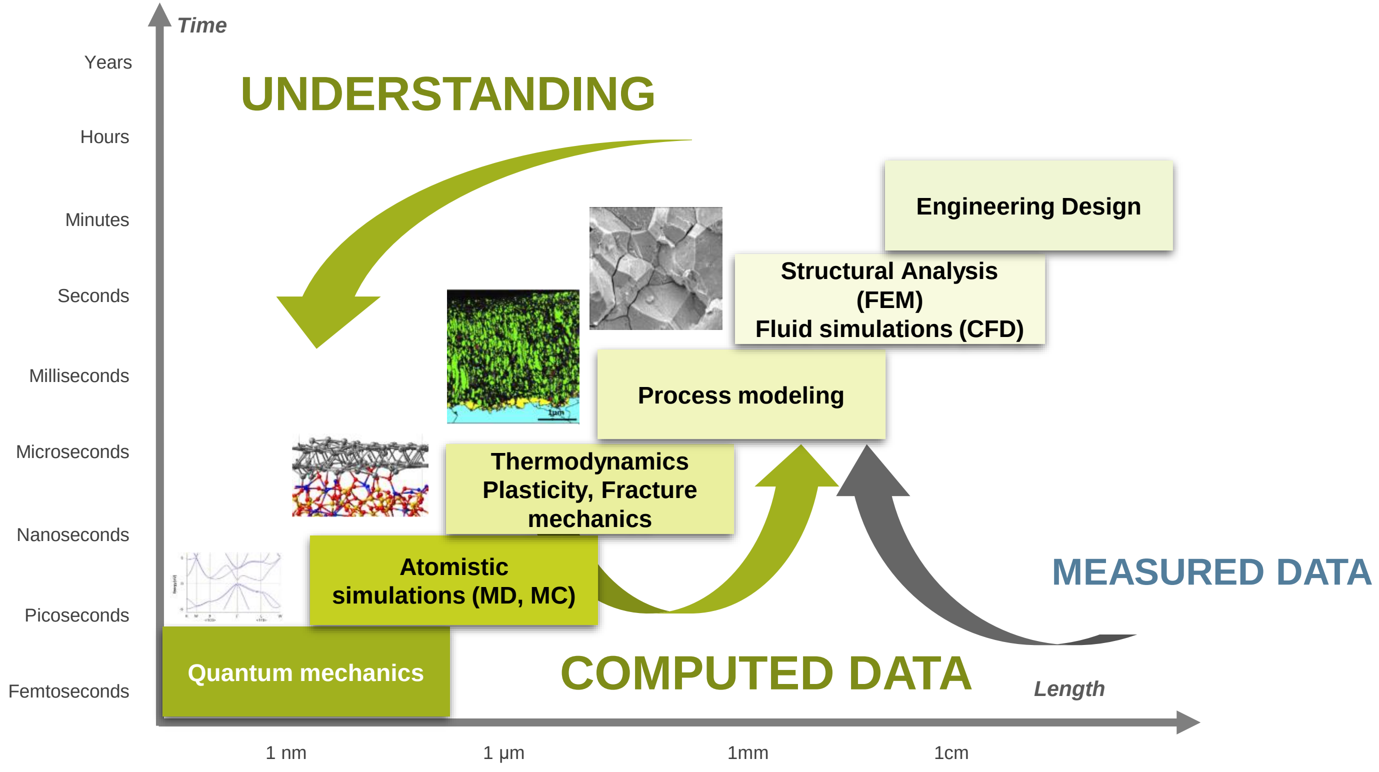
  Scaling Up from Atomistic Simulations to Microstructure Modeling.

Materials Design Company Profile

Established Legacy:	Since 1998. Serving 700+ institutions worldwide.
Our Mission:	Creating Engineering Value from Materials Simulations.
Offerings:	MedeA® software, support, consulting, and contract research.
International Presence:	Headquartered in San Diego, USA, and Paris, Europe.
Partnerships:	Collaborating with technology and business partners globally.
Expertise:	Computational materials science, chemistry, chemical engineering.



Improved Decision-Making Through Data And Understanding



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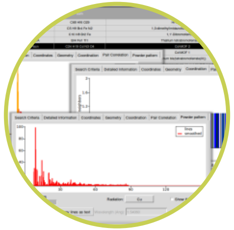
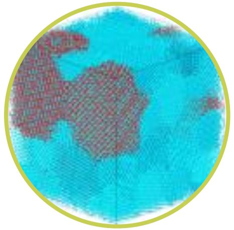
MedeA Environment



Databases

Experimental structures and properties,
ICSD, Pearson,, COD, Eureka



Builders

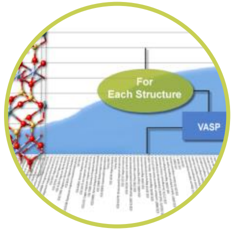
Models: molecular, fluid, solid,
nano, micro, …

Engines

VASP, LAMMPS, GAUSSIAN, GIBBS, MOPAC …

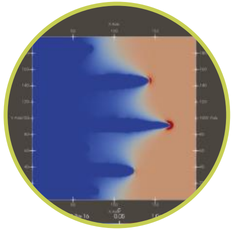
Automation

Properties: thermal, mechanical, transport, phase stability, …



High Throughput

Workflows, structure lists,
Job control, local, cloud



Analysis

Structure-property, graphical,
machine learning

Combines experimental data, builders and compute engines with automation high-throughput, and analysis

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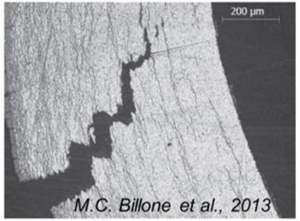
Corrosion

The cost of corrosion is estimated at 3.4% of the global GDP

- Water-cooled nuclear reactors: Corrosion of cladding of fuel rods is a life-limiting degradation mechanism
- Oil & Gas: Corroding pipelines drive up costs
- Automotive: Poor corrosion resistance of Magnesium alloys prevent lighter cars



Can we simulate corrosive processes over days/months/years and make predictions?

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Zirconium Corrosion And Hydride Formation In Reactors

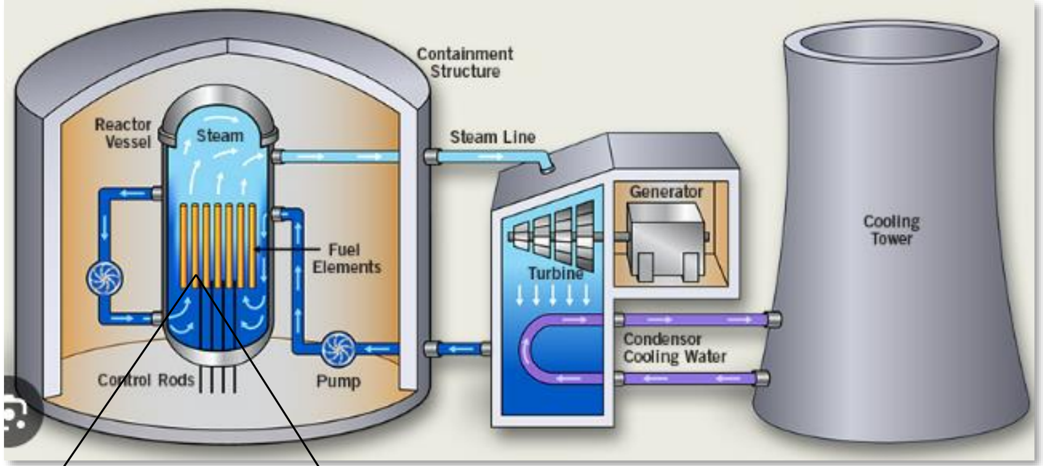
- Water reacts with Zr cladding of fuel rods, freeing hydrogen

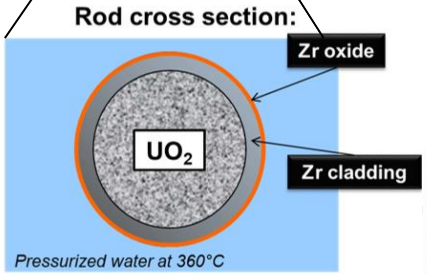
Corrosion reaction:

$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2$$

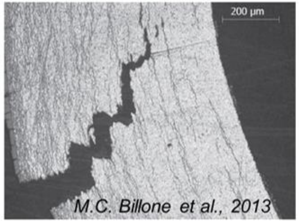
- Formation of Zr hydride
- Hydrogen embrittlement and mechanical weakening

How does the hydride microstructure look for a given H influx, temperature, and material?





Hydrided Zr cladding



Modeling Corrosion of Zirconium Alloys Fuel Cladding – The UW-Madison Materials Degradation under COrrosion and Radiation (MADCOR) – UW–Madison (wisc.edu)

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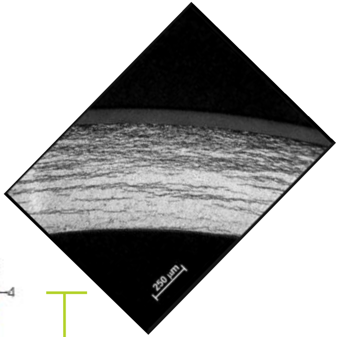
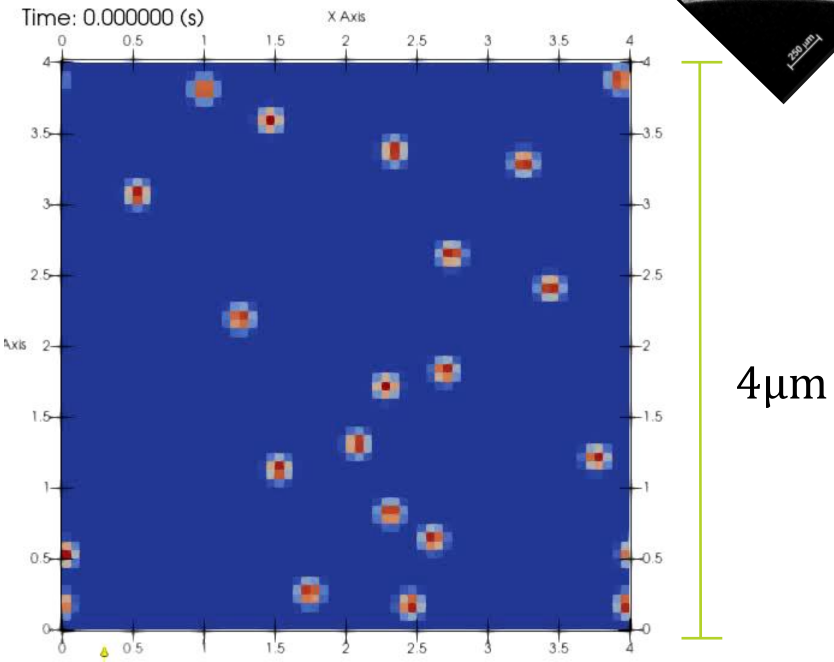
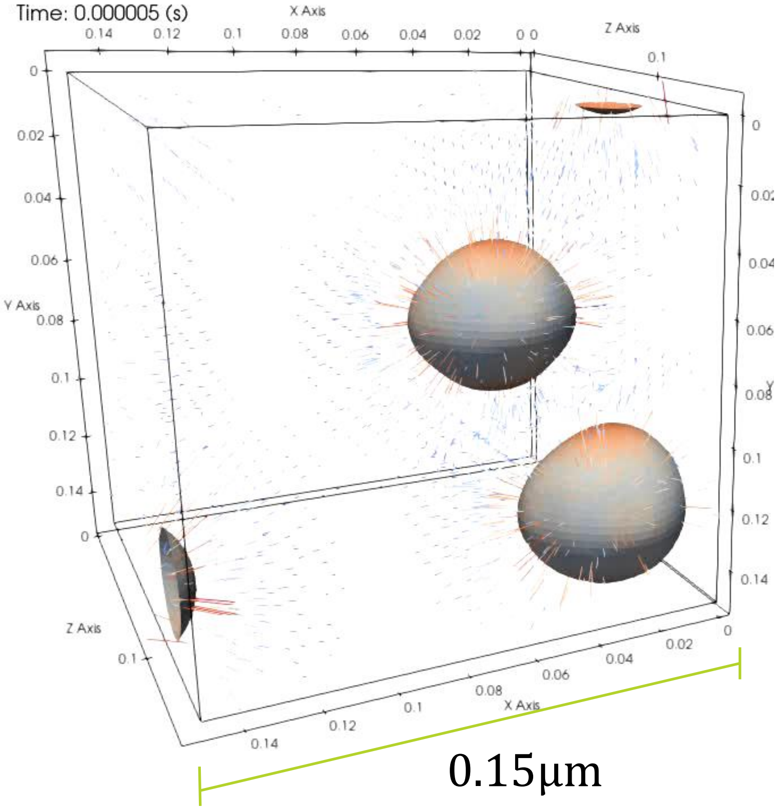
Hydride growth







Zr and hydride phase evolution (for 0.07s at 600K) shows effect of elastic anisotropy

3D simulation with H fluxes and elastic energy at interfaces

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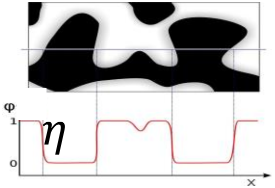
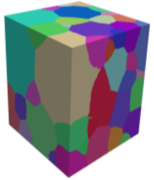
From Nanoseconds To Years

Atomistic simulations

Machine Learning Potentials

Microstructure evolution

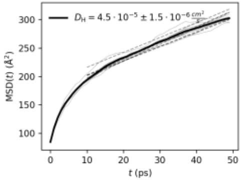
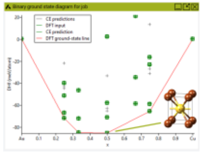
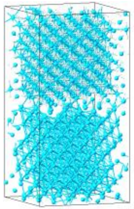
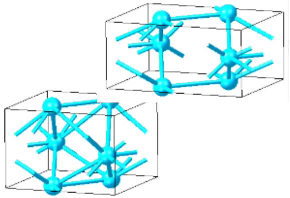




$$F = \int dV\,[f_{chemical} + f_{interface} + felastic]$$

$$\frac{\partial c}{\partial t} = \nabla\, \mathrm{M}(c, \eta, \sigma) \nabla \frac{\delta F}{\delta c}$$

$$\frac{\partial \eta}{\partial t} = -L \nabla \frac{\delta F}{\delta \eta}$$

Diffusion	Free energy	Interfaces	Elastic energy
			

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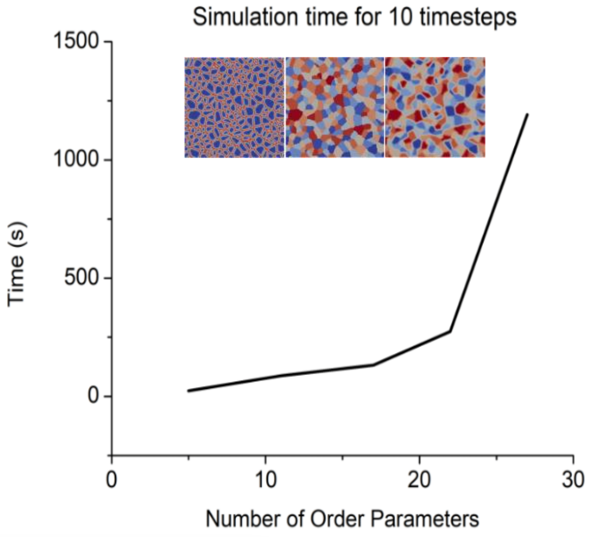
Summary

- Safety, economy, and sustainability of primary energy generation are major challenges of this century
- Understanding corrosion and material degradation requires multi-scale modeling
- Multi-scale simulations require
  - Accurate and efficient computations of chemical, thermo-mechanical, interfacial, and transport properties
  - Machine-learned potential for scale-up and complexity
  - Realistic 3D Microstructure simulations with the above input
  - Significant parallel computing resources

Phase field



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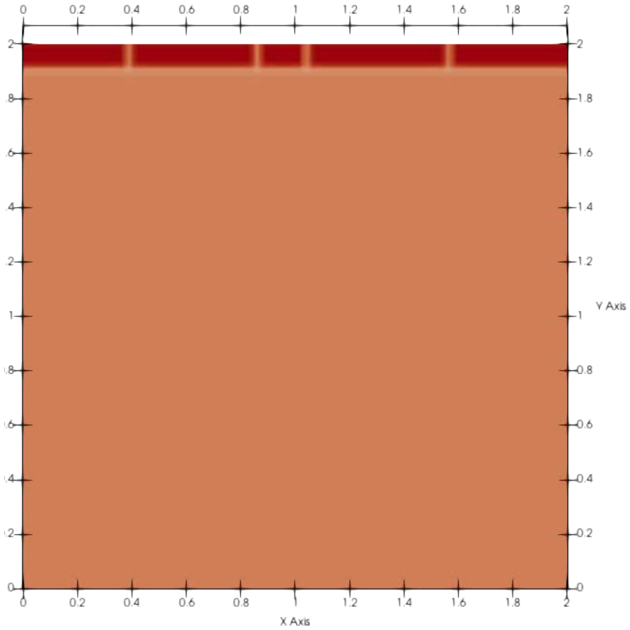
More Examples

Crack formation in α-Zr – m-ZrO_2 and Mg – MgO

Cracking In Materials With Different Pilling-Bedworth Ratios

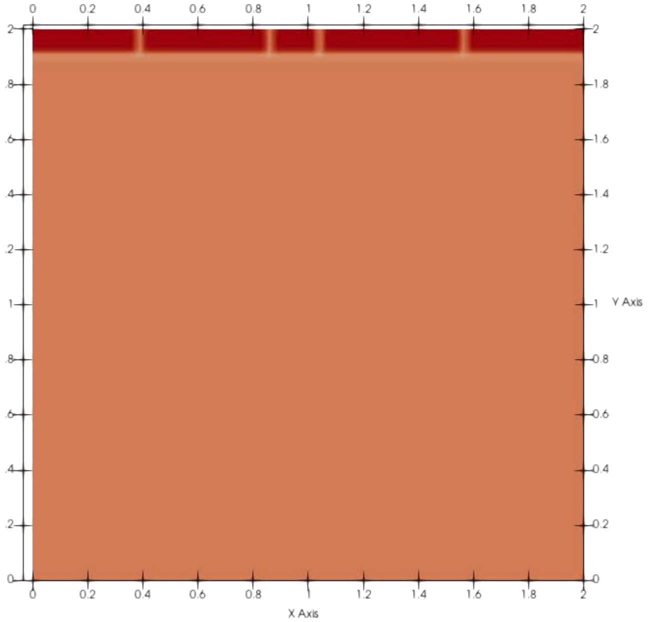
$$PBR = \frac{V_{oxide}}{V_{metal}}$$

Zirconium oxide PBR: 1.56



Cracks forming in a α-Zr – m-ZrO_2 multi-grain simulation at high O flux

Magnesium oxide PBR: 0.81



Cracks forming in a Mg – MgO multi-grain simulation at high O flux

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Optimising Ignitor Beam Properties in Proton Fast Ignition

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

Project: *"EHPC-REG-2023R01-043"*

EuroHPC used: Vega, Karolina

Speaker: Paul *GIBBON (Focused Energy)*

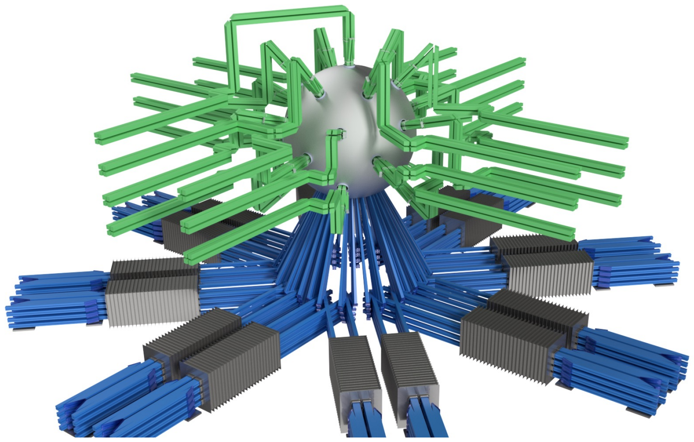
Focused Energy was founded in July 2021

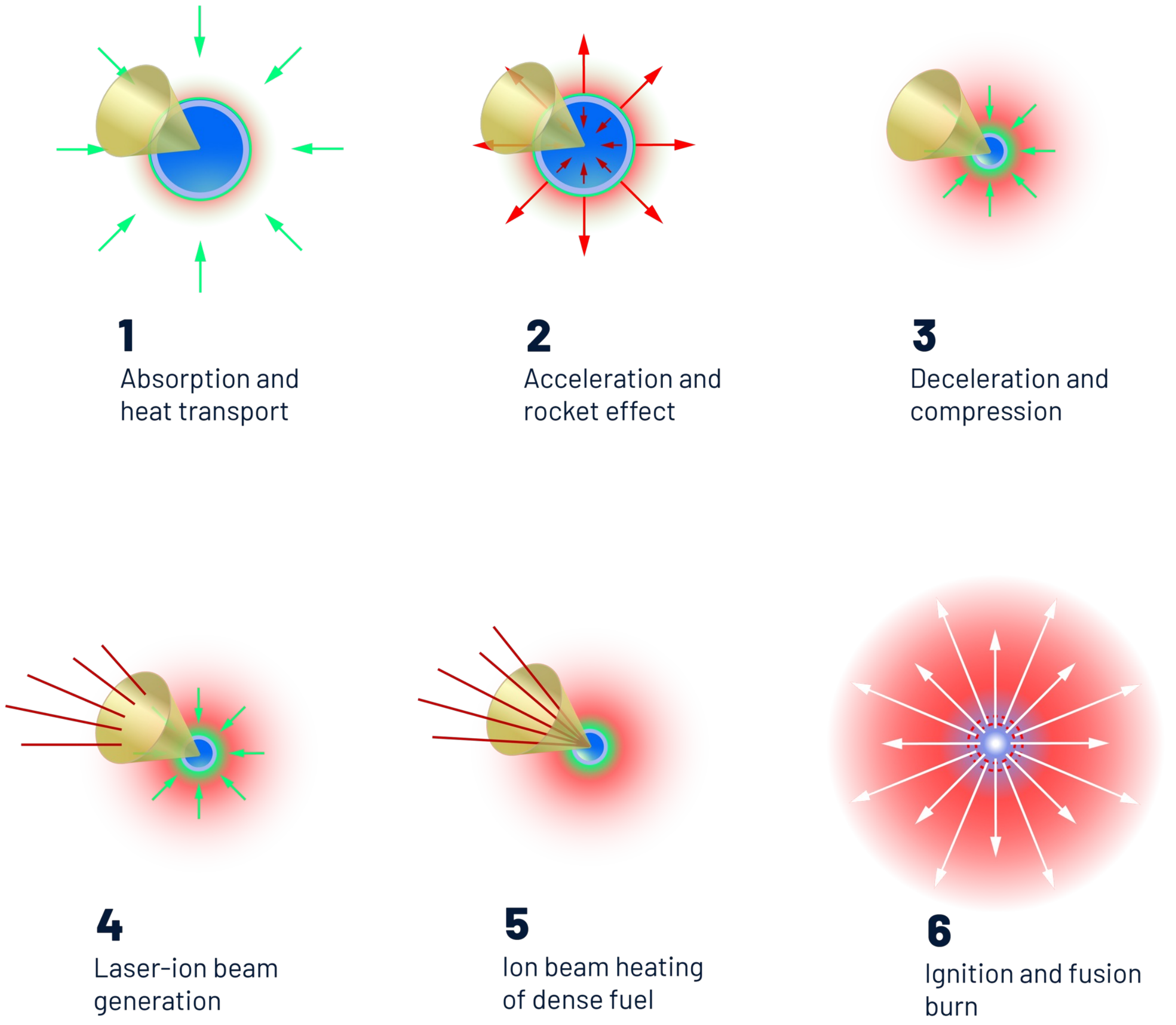
Our goal: demonstrate commercially viable inertial fusion energy

Laser-driven fusion with the Proton Fast Ignition scheme*

The Proton Fast Ignition (PFI) concept comprises several distinct steps:

- long-pulse laser driver absorption by the plasma (1)
- fuel compression (2-3)
- short-pulse laser generation and transport of a proton beam (4-5)
- fuel ignition and burn (6)

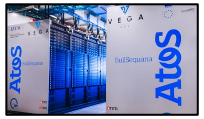


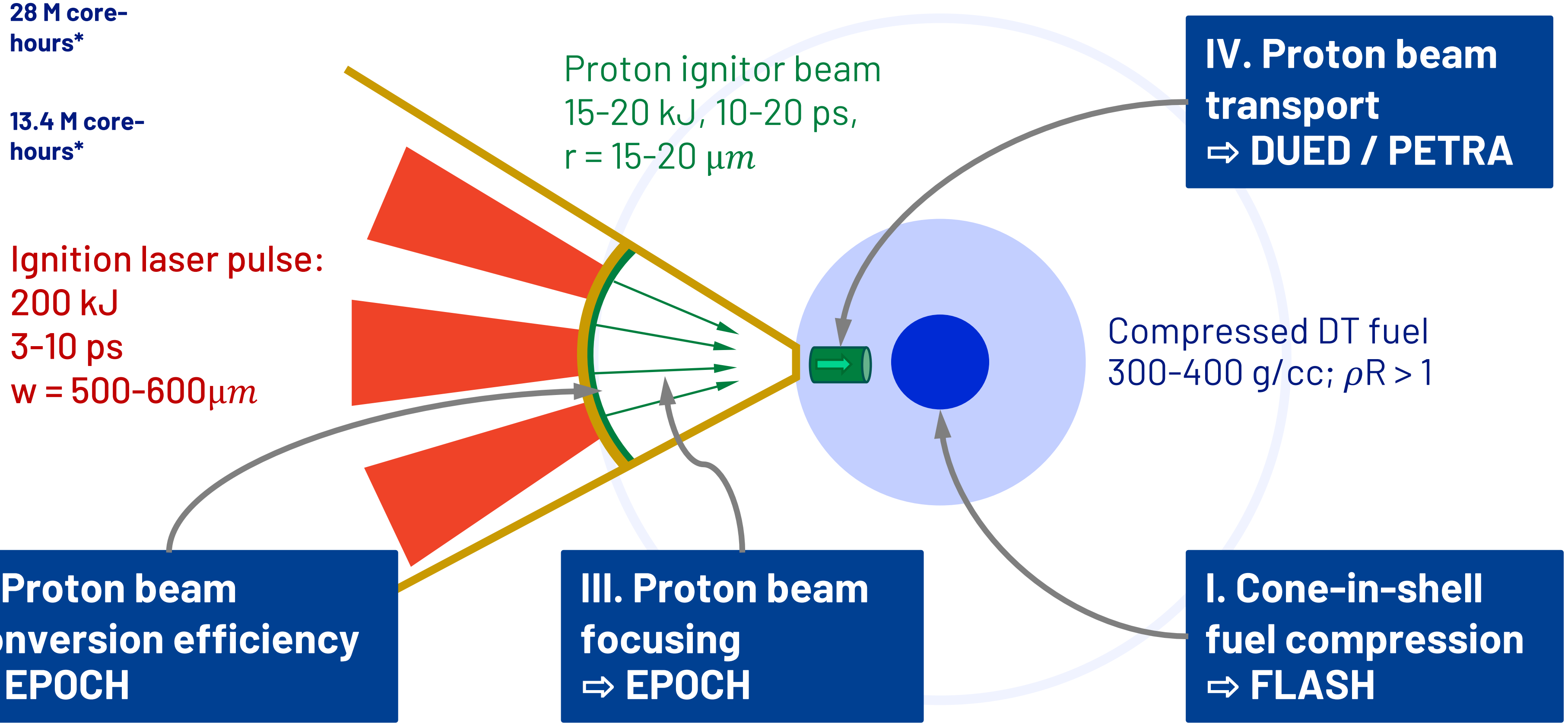


*M. Roth et al., PRL 86, 436 (2001)

HPC access through EuroHPC is helping FE to tackle key computational design challenges

FOCUSED ENERGY

	HPC Vega, IZUM, Maribor	**28 M core-hours***
	Karolina supercomputer IT4Innovations, Ostrava	**13.4 M core-hours***



EuroHPC project: EHPC-REG-2023R01-043

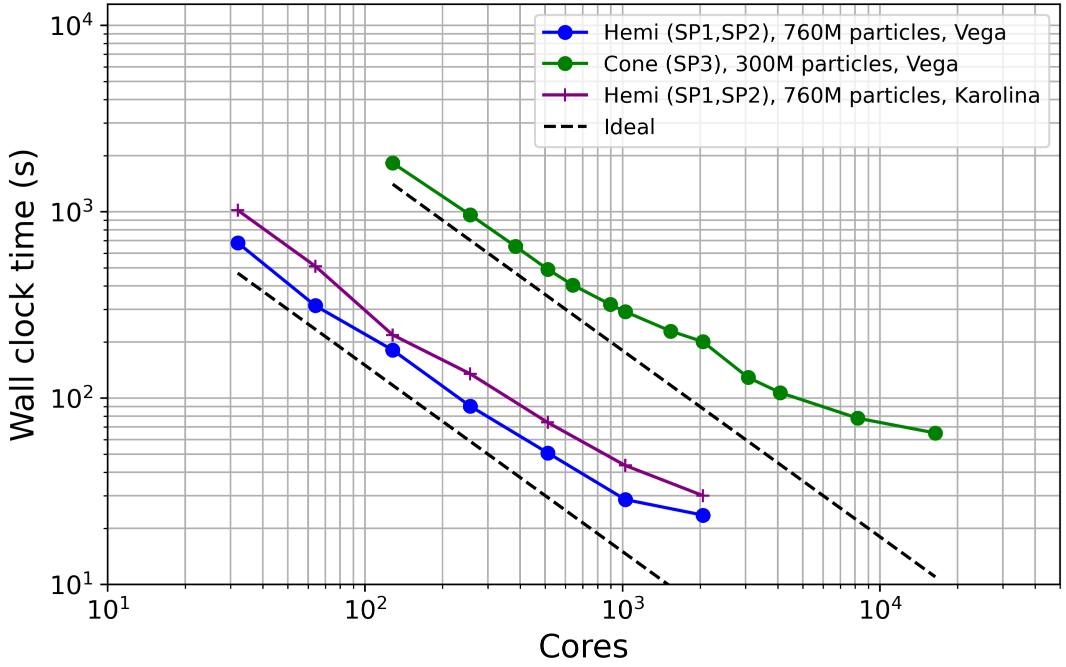
EuroHPC Joint Undertaking

Performance of EPOCH and FLASH codes on Vega & Karolina

FOCUSED ENERGY

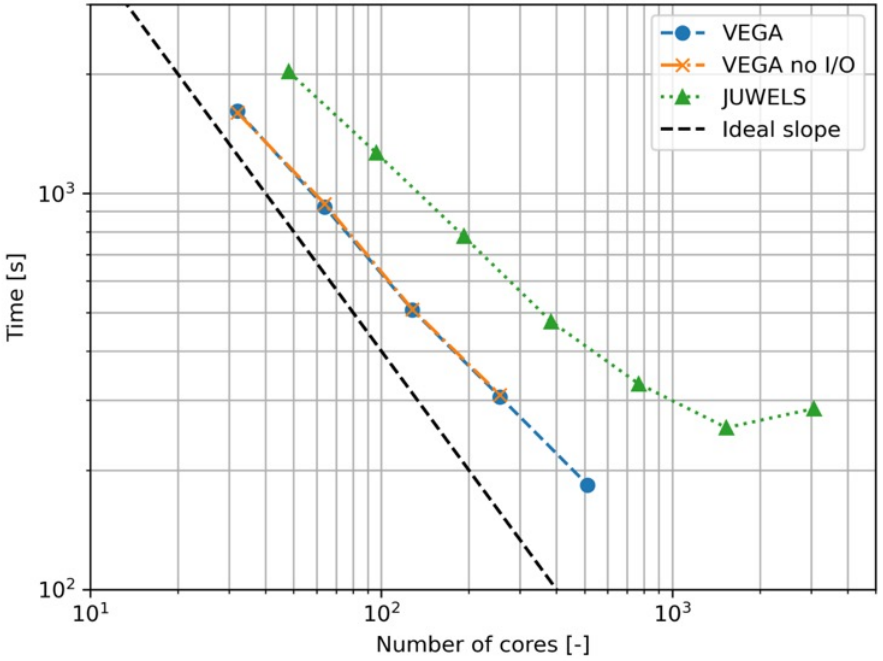
EPOCH

T. Arber et al., PPCF ***57****, 113001 (2015)*



FLASH

B. Fryxel et al., Ap J. ***131****, 273 (2000)*



- Both codes exhibiti good weak scaling, so feasible to run with 10B particles/grid points on >10^4 cores
- CPU, MPI only (OpenMP possible). Other PIC codes available exploiting GPU, parallel I/O libraries

I. Cone-in-shell simulation of DT fuel compression with FLASH

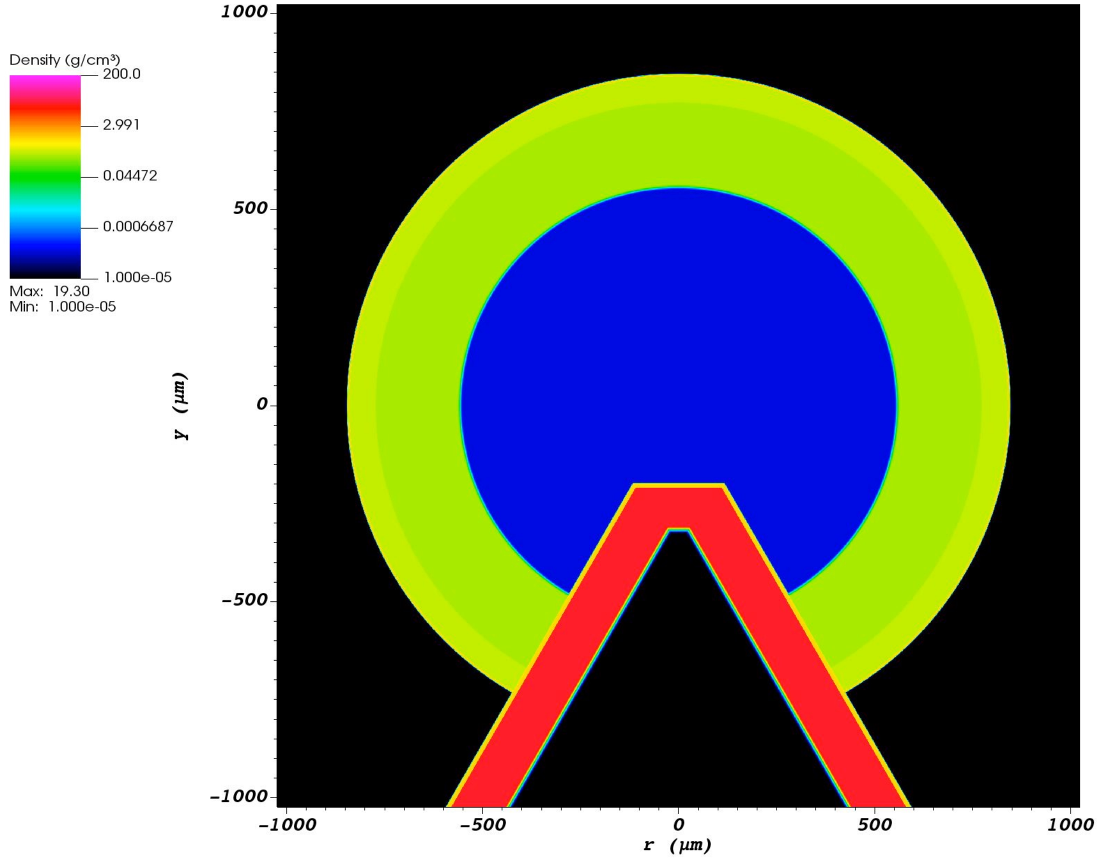
Alfonso Mateo Aguaron, Javier Honrubia (UP Madrid & FE)

Simulation details:

- 2D cylindrical geometry for hydro & laser ray-tracing
- Grid domain 1024 μm x 2048 μm; AMR with 1 μm resolution, blocksize 16x16
- Variable timestep Δt = 1.3e-13 s; 20h runtime on 512 cores

Mitigation of FLASH technical issues:

- grid remapping to remove numerical Rayleigh-Taylor instabilities
- corrected equation of state to avoid negative pressures etc.
- smoothing across material interfaces
- calibration of shock wave propagation via cross-code benchmarking with MULTI-IFE and DUED



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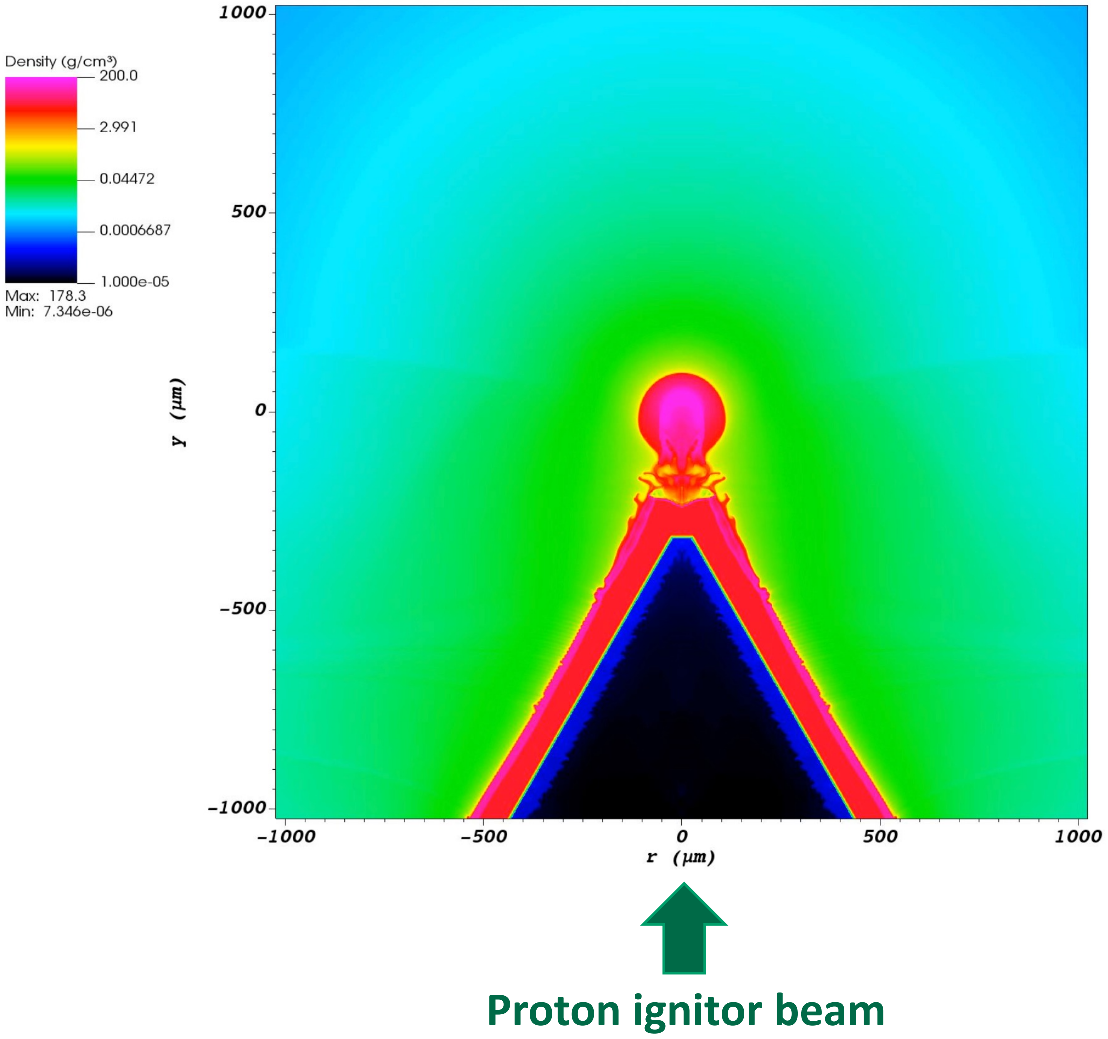
- smoothing across material interfaces
- calibration of shock wave propagation via cross-code benchmarking with MULTI-IFE and DUED



II. Proton beam conversion efficiency (CE) modelling

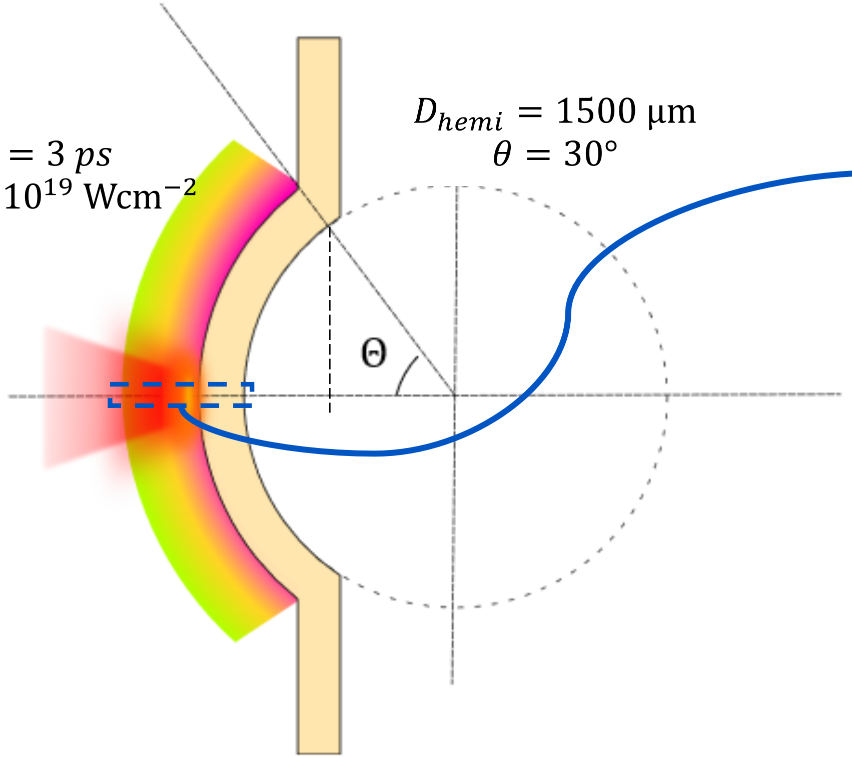
Valeria Ospina-Bohorquez

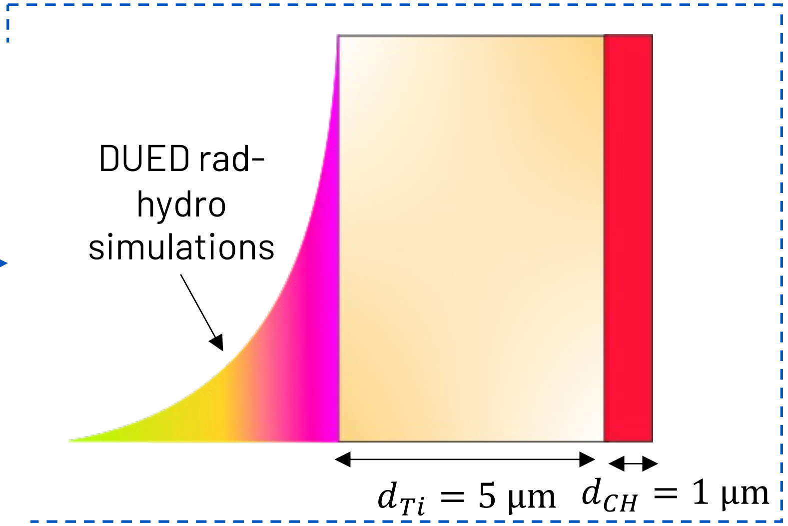
Laser parameters:

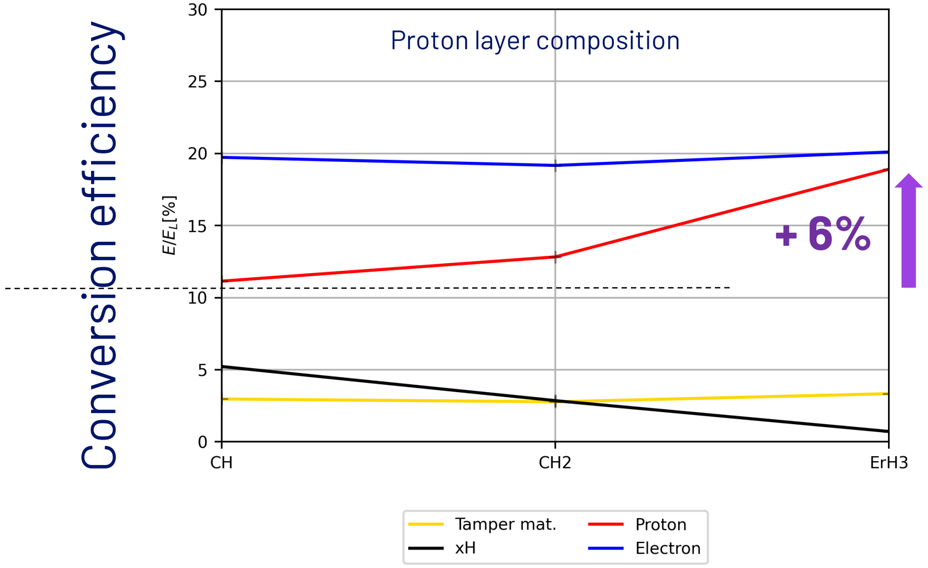
- intensity
- contrast
- duration, shape
- spot size, distribution
- wavelength?

Target parameters:

- substrate thickness
- proton layer thickness
- proton layer composition (LiH, CH_n, ErH_3 …)*



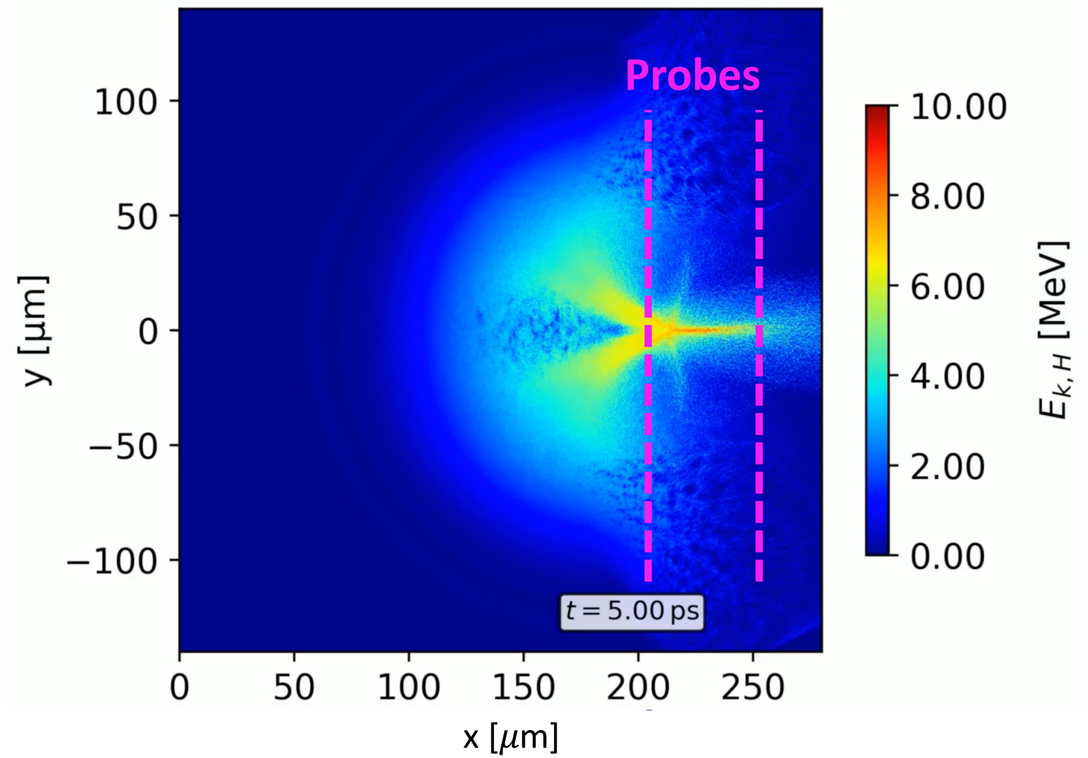


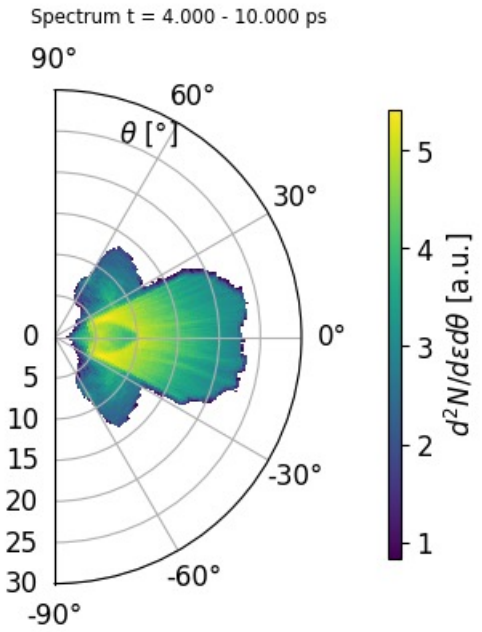


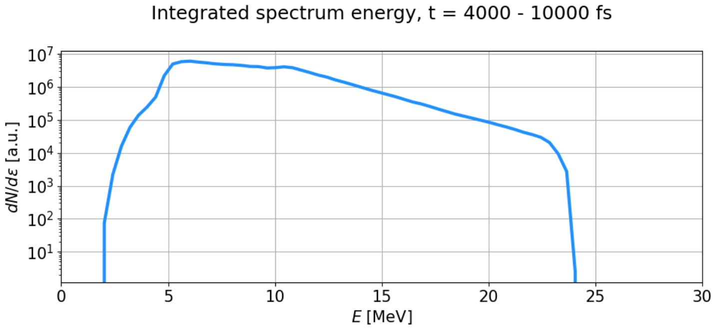
- At today's prices, each 1% improvement in CE translates to saving of ~ $50M in the ignitor laser system!

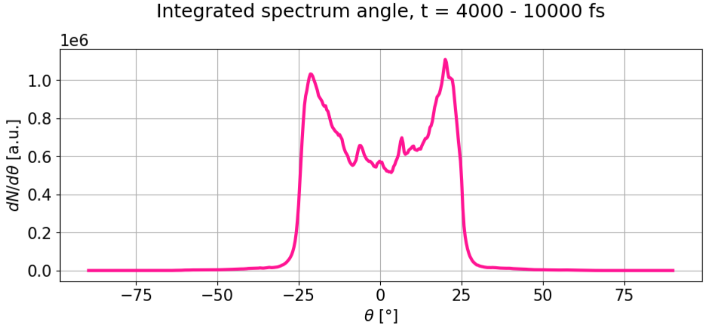
2-D simulations with diagnostic probes to characterize proton beam

FOCUSED ENERGY





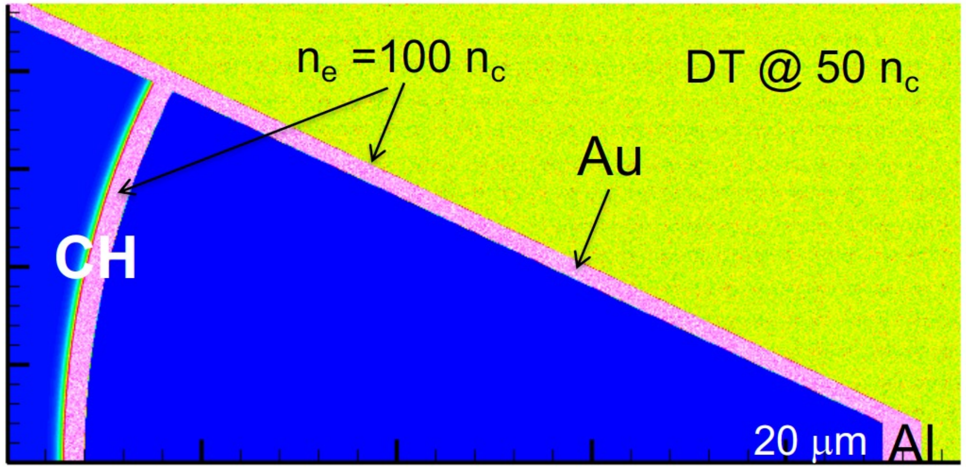


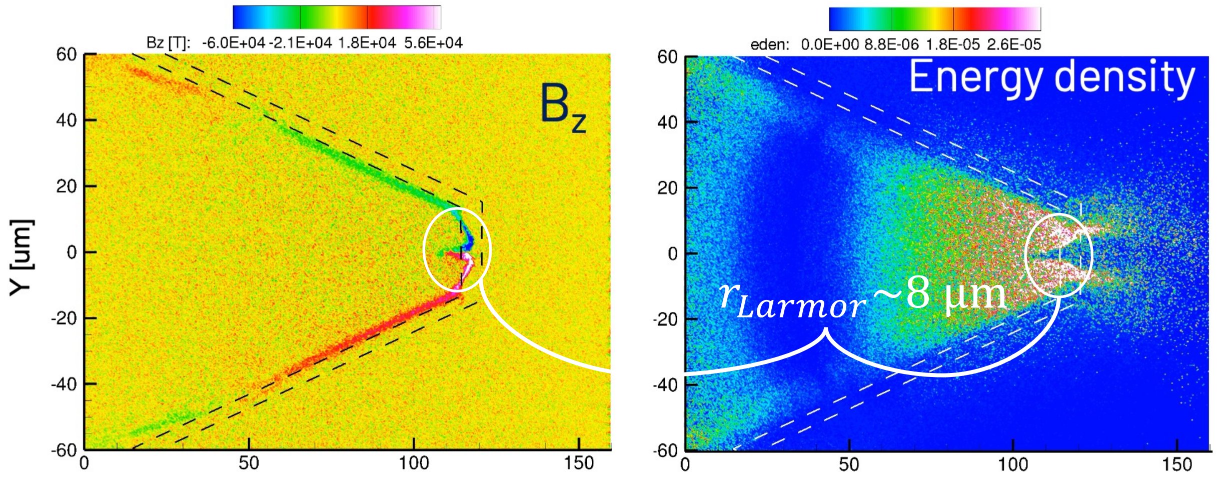


- Upcoming experimental campaign on proton focusing in spring 2024 at Colorado State University (LaserNetUS Program)

III. Proton beam focusing with ‘integrated’ cone targets*

Javier Honrubia





Multiple effects of cone wall and DT fuel plasma:

- Strong *return currents* through cone walls and from DT plasma replenish foil electrons and suppress sheath field, reducing proton conversion efficiency
- Magnetic fields generated near cone tip cause strong proton *beam defocusing*
- Mitigation measures: reduced laser intensity, double cone walls, heavy ions
- Does the cone-tip B-field & defocusing effect still persist for mm-scale cones?

Honrubia, Morace and Murakami, MRE **2, 28 (2017)*

*Recent expt: King et al., PPCF **66** 015001 (2024)*

Putting the pieces together for ignition-scale targets

Novel features:

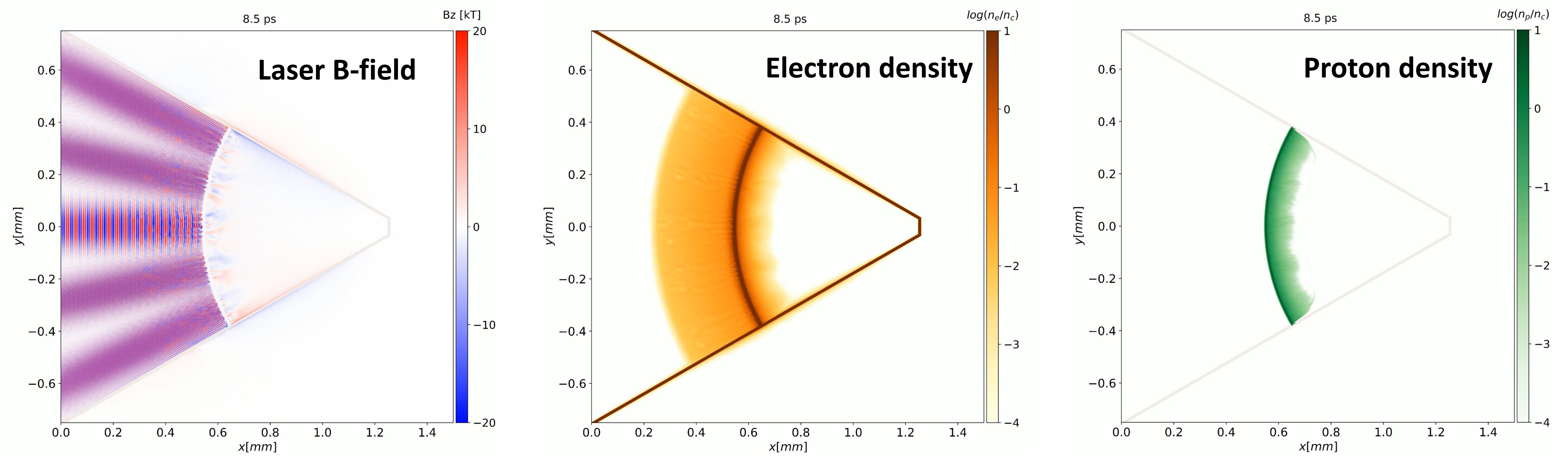
- Multi-beam laser irradiation in mm-scale cone geometry: 5 x $I_L = 3.0 \times 10^{19}$ Wcm^{-2}; $\lambda = 1\ \mu m$; $\tau_L =$ 3ps; $\sigma_{FW} = 100\ \mu m$
- Utilize 'best of' parametric target scans: rad-hydro computed pre-plasma, laser profile, foil composition & dimensions

Numerics:

- 30k x 30k = 9 x 10^8 grid points; $\Delta x = \lambda_L/20$
- 2 x 10^9 particles
- 36h on 3k cores of Vega

Future refinements:

- collisions, ionization, wall isolation, 3D!



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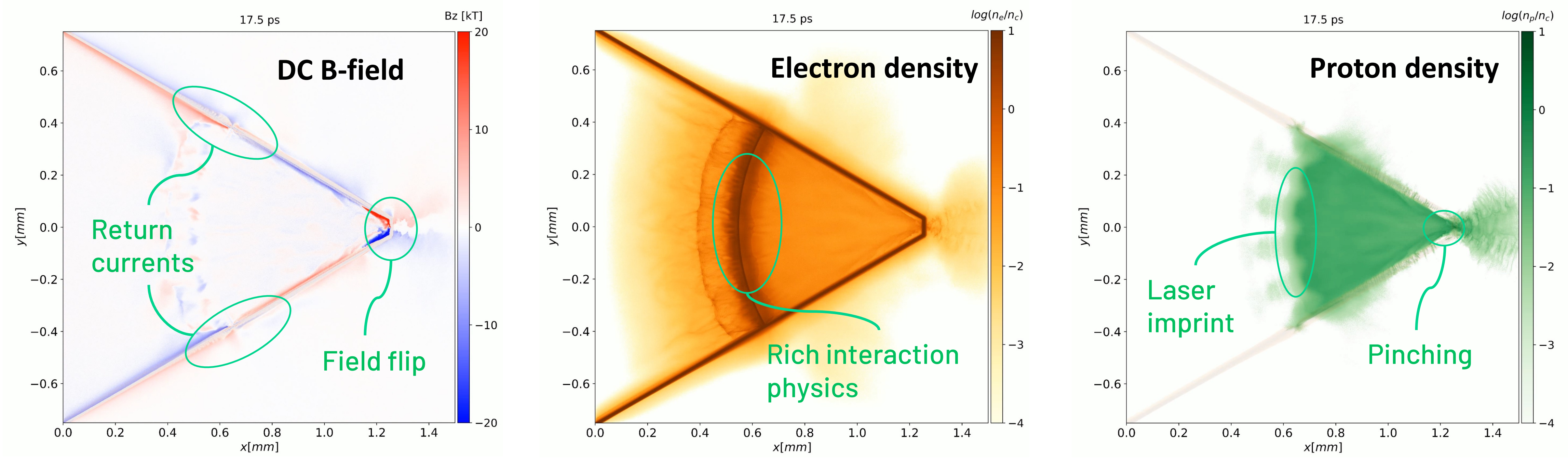


IV. Proton beam divergence leads to higher ignition threshold

FOCUSED ENERGY

Javier Honrubia

PETRA hybrid code*:

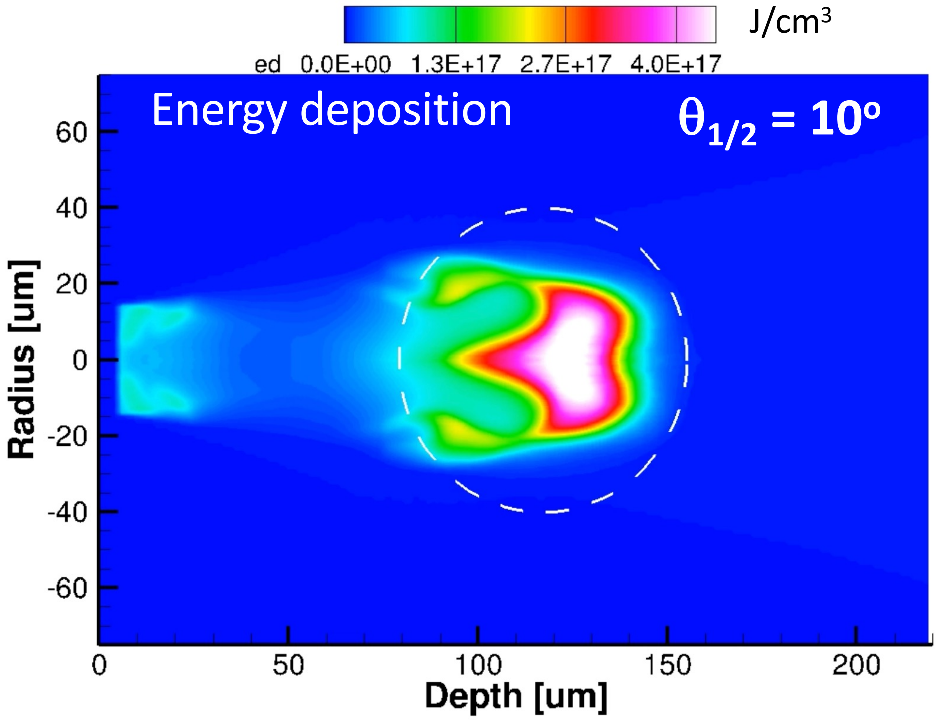
TNSA proton beam with T_p = 5 MeV transported into **imploded DT**

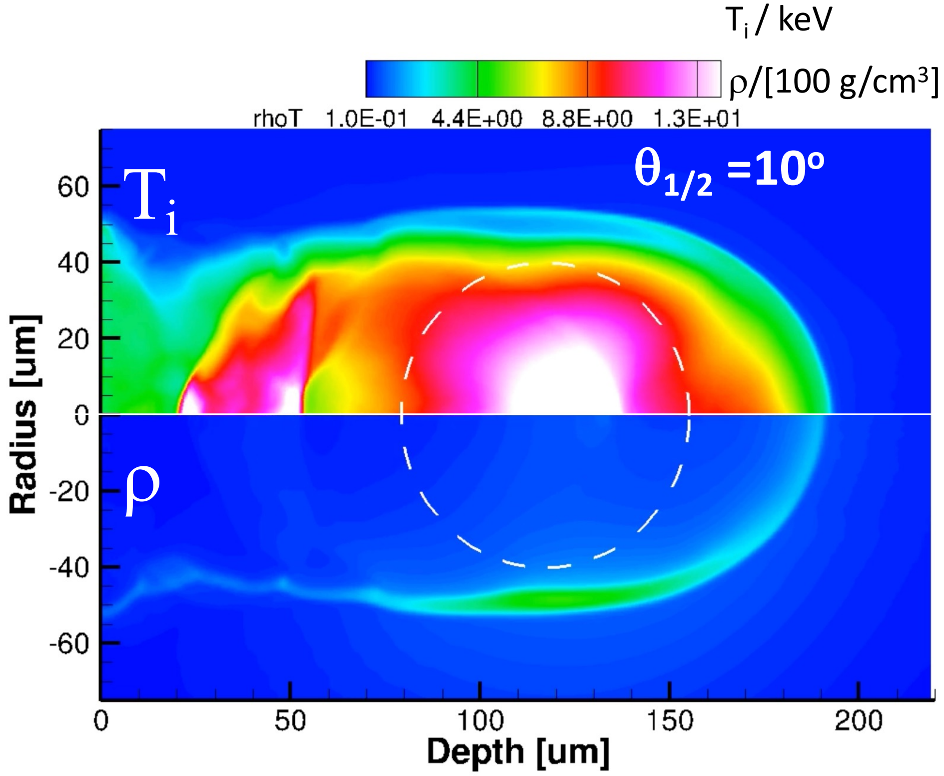
ρ_{max} = 512 g/cm^3

standoff distance = 1 mm

E_{ig} = 18 kJ , $\theta_{1/2}$ = 0º

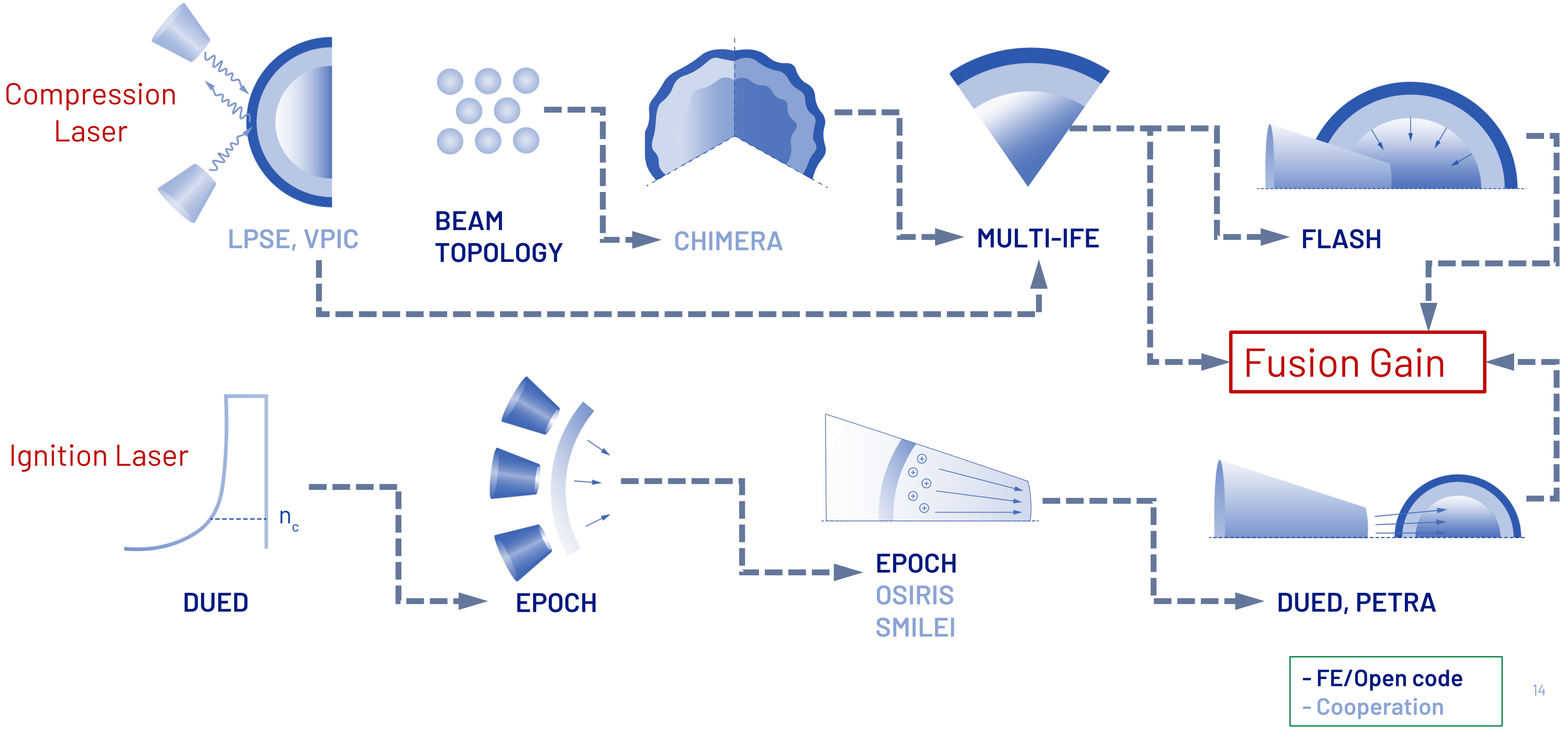
E_{ig} = 27 kJ , $\theta_{1/2}$ = 10º





*See, eg: Honrubia and Murakami, Phys. Plasmas **22**, 012703 (2015)

Towards an integrated PFI model framework



Summary

- **Progress on key open physics questions of Proton Fast Ignition:**
  - Isochoric compression of DT fuel capsule with inserted cone
  - Options identified for enhancing proton beam conversion efficiency
  - Proton beam focusing in full-scale cone targets: control of return currents
  - Heating and ignition of compressed DT fuel: sensitivity to beam properties

- (Pre-) exascale computing resources (100s of millions of core-h) will play a vital role in de-risking inertial fusion power plant design

- Future sub-scale, high repetition-rate experimental facilities will enable quantitative calibration and refinement of models

Thanks to ...

EuroHPC JU for awarding this project access ***EHPC-REG-2023R01-043*** hosted by VEGA, Maribor and KAROLINA, Ostrava

and

The Focused Energy Science Team:

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