Richard More, *LBNL HIF-VNL, LLNL*

Particle simulation of fusion ignition

Original ideal: *calculate everything with MD*

electrons	==>	$\log \Lambda$	
DT ions	==>	$f(E)$	with no approximation
radiation	==>	I_ν	

Test standard formulas for plasma processes
Clairvoyant diagnostic of fusion ignition phenomena
Test ideas for new experiments

Two difficulties:

1.) **Time-steps and code speed**

To see ignition, must run for ~ 10 psec = **10^{-11} sec**
To resolve e-i collisions, need time-step **dt < 10^{-22} sec**
It is possible to take **10^6 time-steps**
but we need strategy to achieve **dt = 10^{-17} sec**

Analytic formula for binary Coulomb collision ($\theta > 2^\circ$)
Weakly-coupled plasma <--- $\Gamma \leqq .01$ at ignition conditions
e-i coupling by a Langevin method (use *log* Λ, don't predict it.)
Subcycle the fusion alphas, supercycle the Langevin steps

2.) **QM Processes in a classical simulation**

Need quantum treatment for **fusion, radiation**
During the simulation, Classical ---> Quantum --> Classical

Conditional probabilities (Small-ball method) MD / MC hybrid

PARTICLE SIMULATION METHODS

PIC = Particle-in-cell = representative particles with fields on grid
Appropriate for "macroscopic" phenomena

QMD = Quantum molecular dynamics = DFT electrons + classical ions
Appropriate for low-temperature (WDM) conditions

MD = Molecular Dynamics = classical point particles

MD ions have $\{R_i\}, \{V_i\}$

Arbitrary f(E) "self-regulated" by { ion-ion collisions, ion energy-loss, tail-filling }

For fusion, MD + quantum effects treated by MC method

NEW: Reactions change the particles D + T --> α + n

ELECTRONS ==> *FLUID* n_e, T_e

==> Big benefit for code time-step

Ion coupling to electrons by a ***Langevin method***

Many ei collisions during dt combine as a random walk.

During time dt, probability that ion changes velocity by d**v** is

$$P(d\vec{v},\vec{v}_i,dt) = \left(\frac{M_i\tau}{2\pi kT_e dt}\right)^{3/2} e^{-\frac{M_i}{2kT_e}\frac{\tau}{dt}(d\vec{v}+\gamma\vec{v}_i)^2}$$

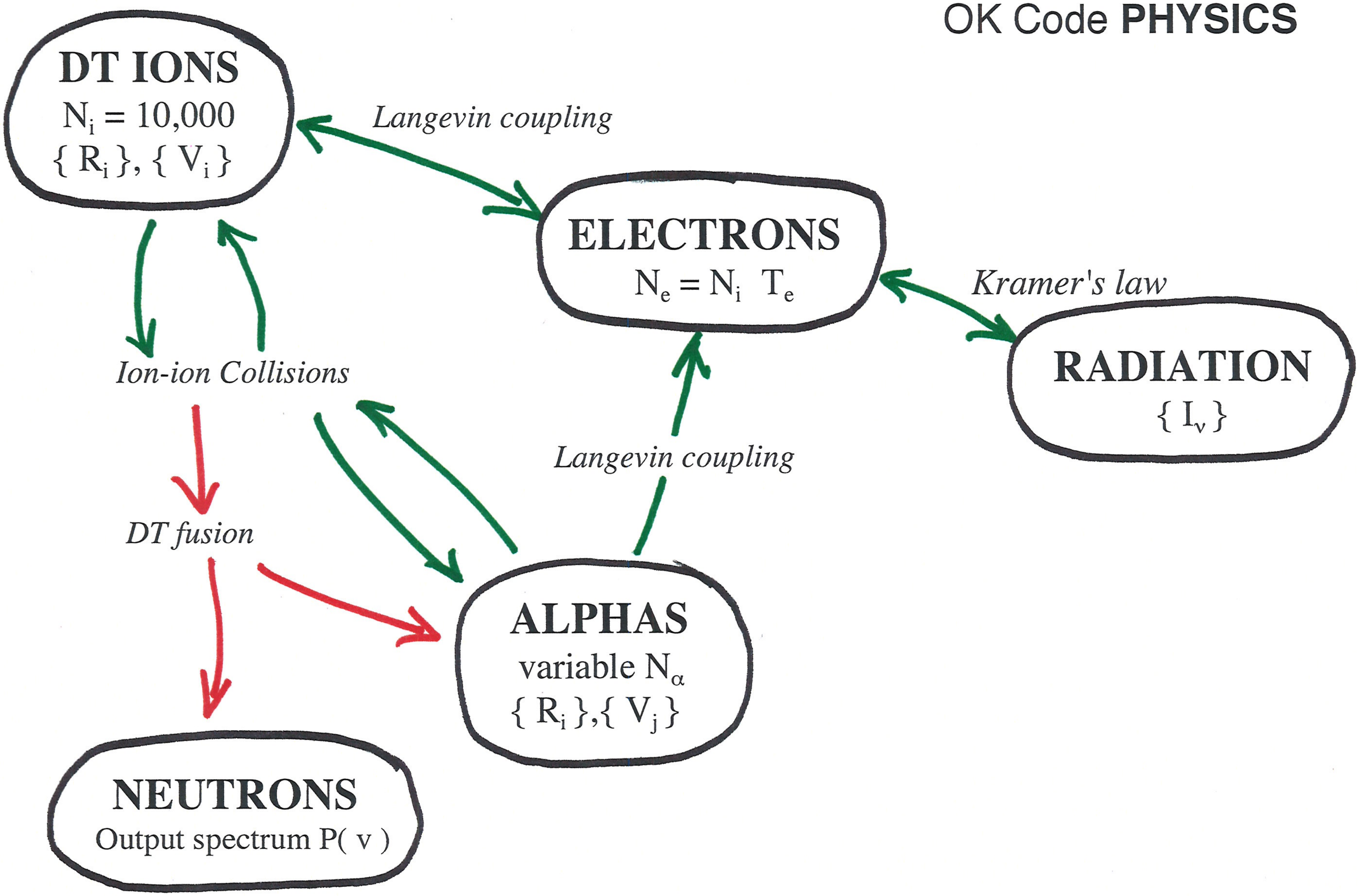
Chandrasekhar

Average $< d\mathbf{v} > = -\gamma\,\mathbf{v}_i$ describes ion *dE/dx* to electrons; $\gamma = dt / 2\tau$

Landau-Spitzer-Longmire formula for τ :

$$\frac{1}{\tau} = \frac{8\sqrt{2\pi}}{3}\frac{Z^2e^4n_e}{M_ikT_e}\sqrt{\frac{m_e}{kT_e}}\left(\frac{m_e}{m_r}\right)\log\Lambda$$

OK Code **PHYSICS**

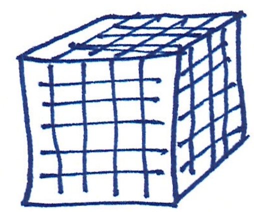


Processes

OK code

Ion-ion collisions	cutoff Coulomb potential
Electron-ion $(dE/dx)_e$ and τ_{ei}	Langevin coupling
Radiation emission, absorption	Kramers' formulas
Fusion reactions	small-ball method $P_c = \sigma_{DT} / (\pi R^2)$
Alphas: ion collisions, dE/dx to electrons	Langevin coupling

Code structure



Periodic BC on simulation box

$(15)^3 = 3375$ sub-boxes, ~ 3 ions in each

Pointers: ion--> box, box --> neighbor boxes, box --> ions

"Periodic distance" between two points (shortest way)

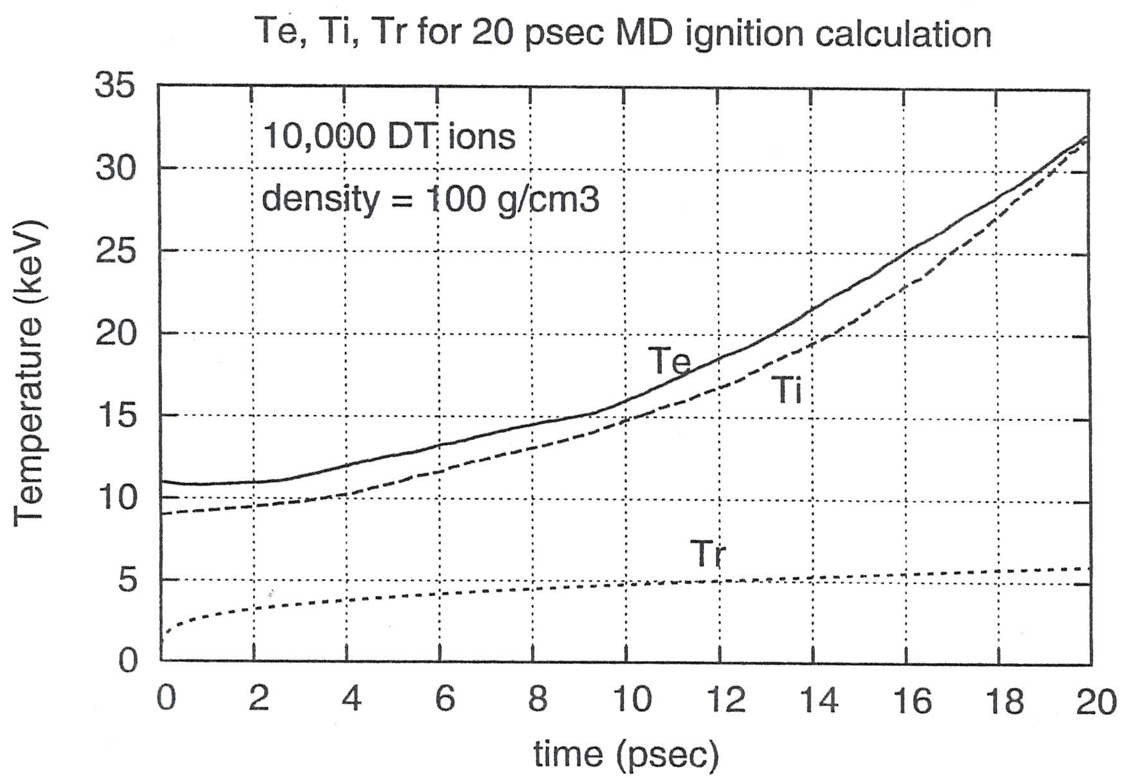
Synchronized subcycle time-steps for alphas

OK code

Ignition simulation with 10,000 DT ions

Temperature rise from 10 keV to 30 keV in 20 psec

316 fusions code run-time ~ 89 hours



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FUSION IGNITION SIMULATION - Typical numbers

10,000 ions (50 % D, 50 % T) Density = 100 g/cm^3 = 2.41 10^{25}/cm^3

Simulation box size = 7.5 A Sub-box size = .5 A (3375 sub-boxes)

R_{sb} = .04 A < --- radius of "small-ball" for collisions

$T_i^0 = T_e^0$ = 10 keV T_r^0 = 1 keV

$v_D \sim v_T \sim 10^8$ cm/sec

Coulomb coupling parameter $\Gamma = Z^2e^2/R_o kT_i$ = .007

Fermi energy = 300 eV $\ll$ kT

Debye Length = 1 A Coulomb log ~ 4.5

Maxwellian after ~ .1 - .2 psec

alpha energy-loss time ~ 2 - 5 psec

Fusion ignition after ~ 10-20 psec

ENERGY CONSERVATION < --- *It's a TEST*

For the 20 psec calculation ($2\ 10^6$ time steps),

Plasma initial energy = 300.04 MeV

Plasma final energy = 1,425.27 MeV

Fusion neutrons = 4,463.73 MeV

(316 fusions at 17.586 MeV each)

Energy discrepancy is ~ 31.79 MeV (= 0.54 %)

If it's loss/gain from algorithms, it's $1.1\ 10^{-8}$ per time step

If it is from the fusions, it's ~ 100 keV per fusion

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TESTS

OK code

- ✓ o Ion-ion collisions relax f(E) to Maxwellian in ~ 0.2 psec
- ✓ o electron-ion Langevin (fixed T_e) relaxes f(E) to Maxwellian in ~ 5 psec
- ✓ o Radiation spectrum relaxes to BB (if T_e is held fixed).
- ✓ o Alpha dE/dx to electrons, ions

LIMITATIONS

weak ion coupling, uniform electrons

==> code is ok above $T_{e,i}$ = 1 keV

Fluctuations ~ $1/N^{1/2}$

10^4 ions, but only 10^2 fusions

Expect numerical fluctuations ~ 1 - 10 %

4 ignition self-heating calculations

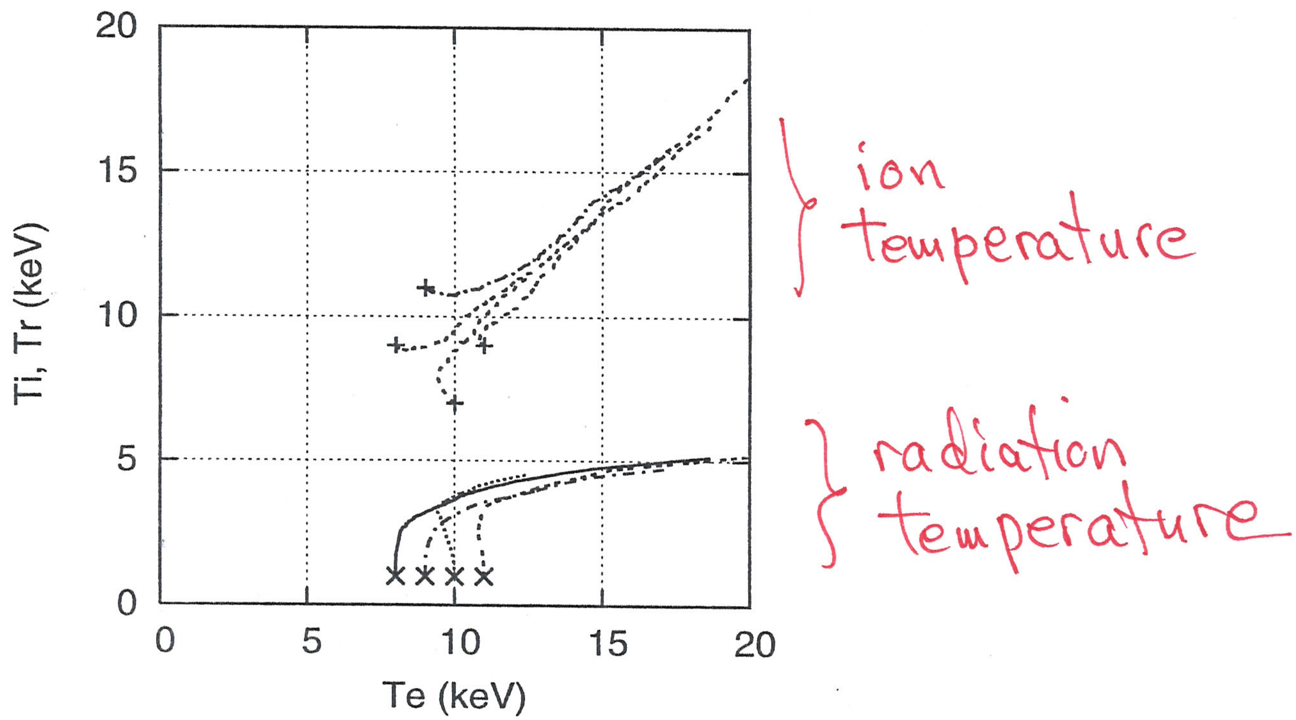
code time	initial T_e^0	T_i^0	final T_e^f	T_i^f	fusions	clock time
15 psec	8	9	18.7	16.6	123	84 h
10 psec	9	11	17.3	15.7	100	60 h
10 psec	10	7	12.5	10.4	45	48 h
20 psec	11	9	32.2	31.9	316	89 h

Wall-clock time may depend on what else was being done on the computer,

but the hot case shows the extra time required to track ~ 300 alphas (subcycled).

Fusion "ignition attractor" phenomenon

- Plasma self-heats along a definite ignition trajectory
- Reliably appears in MD calculations at 100 g/cm^3
- Few psec to join the attractor



Given a fusion particle simulation code, ***what can we do with it?***

--> Non-Maxwell effects in Inertial Fusion ?

--> Ion-beam fast ignition ?

--> "Barydiffusion" ?

--> Novel fusion schemes ?

--> Extend to

MD + Collisional-radiative (atomic model)

(collaboration with F. Wang)

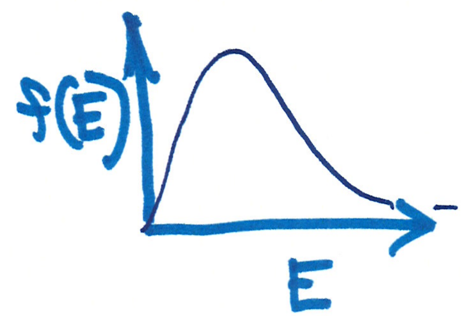
MD + Combustion chemistry

NON-MAXWELL ION DISTRIBUTION

Non-Maxwell ion f(E) from

- Temperature rise too fast for tail-filling
- alphas -- > "knock-on" DT ions
- spatial loss of high-energy DT ions

  Henderson - Petschek - "Knudsen"
- Ion beam heating (FIFI = fast-ion fast-ignition)
- special hydro processes



DT ions certainly thermalize, but

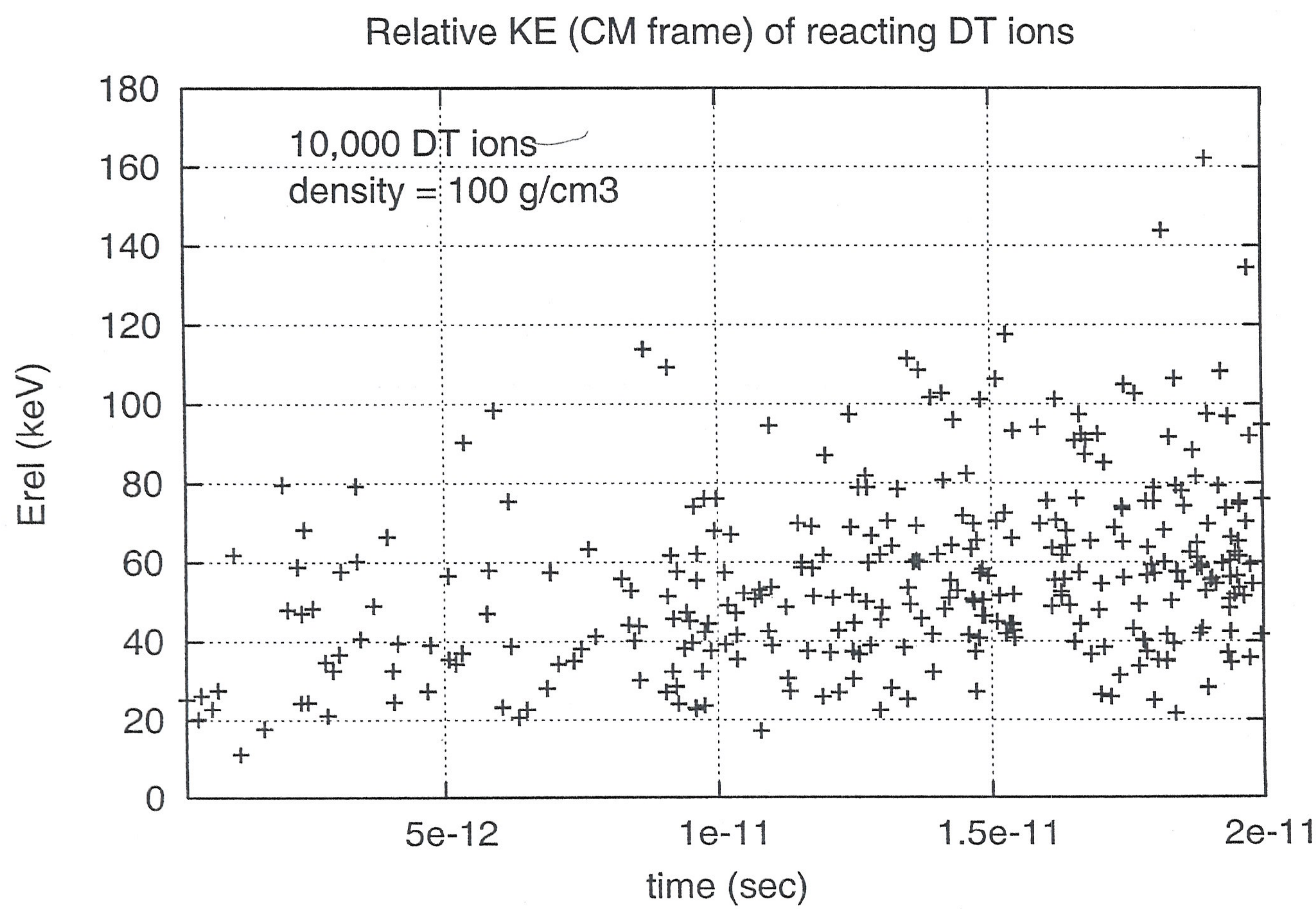
thermalization slow at high E, high T_e

alpha knock-on production increases with T_e

fusion reaction cross-section rises rapidly with E_{rel}

Expect non-Maxwell effects at high temperature

Non-Maxwellian ions affect output **Neutron TOF spectrum**



Relative KE (CM frame) of reacting DT ions
10,000 DT ions
density = 100 g/cm3
Erel (keV)
0
20
40
60
80
100
120
140
160
180
5e-12
1e-11
1.5e-11
2e-11
time (sec)

Neutron TOF spectra

o Output neutron KE has 3 sources: (**v**'s add, not E's)

14 MeV from fusion	+	$\mathbf{E_{rel}}$	+	$\mathbf{E_{cm}}$
Random direction; relativistic E(**v**)		Obtain from the MD for each case Cross-section favors larger E_{rel}		

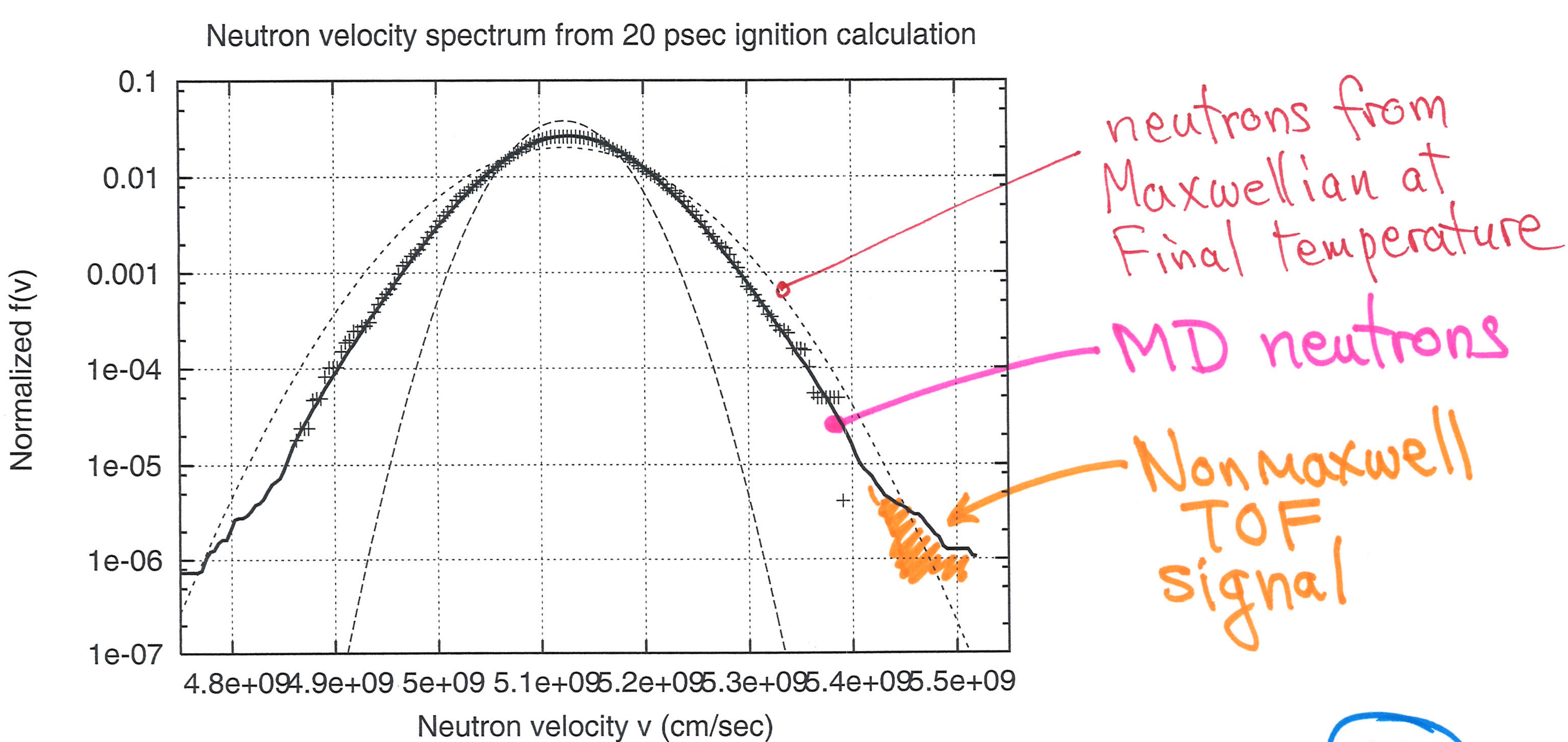
o Calculate output spectrum seen by detectors covering 4π

o Normalize spectrum f(v) to be "per neutron"

Neutrons moving faster than the tail of the final (hottest) Maxwellian are evidence of non-Maxwellian ion f(E) in TN burn.

For a moderately successful ignition experiment, one in 10^6 of the neutrons are predicted to have
velocities ~ .05 10^9 cm/sec *above the hottest Maxwellian.*

At a 10 meter standoff distance, they would arrive ~ 2 nsec early.


Neutron velocity spectrum from 20 psec ignition calculation
0.1
0.01
0.001
1e-04
1e-05
1e-06
1e-07
Normalized f(v)
4.8e+09
4.9e+09
5e+09
5.1e+09
5.2e+09
5.3e+09
5.4e+09
5.5e+09
Neutron velocity v (cm/sec)
neutrons from Maxwellian at Final temperature
MD neutrons
Non Maxwell TOF signal

HIF IGNITION THRESHOLD

100 g/cm^3 DT fuel at $T_e = T_i = 3$ keV <-- this would ignite slowly

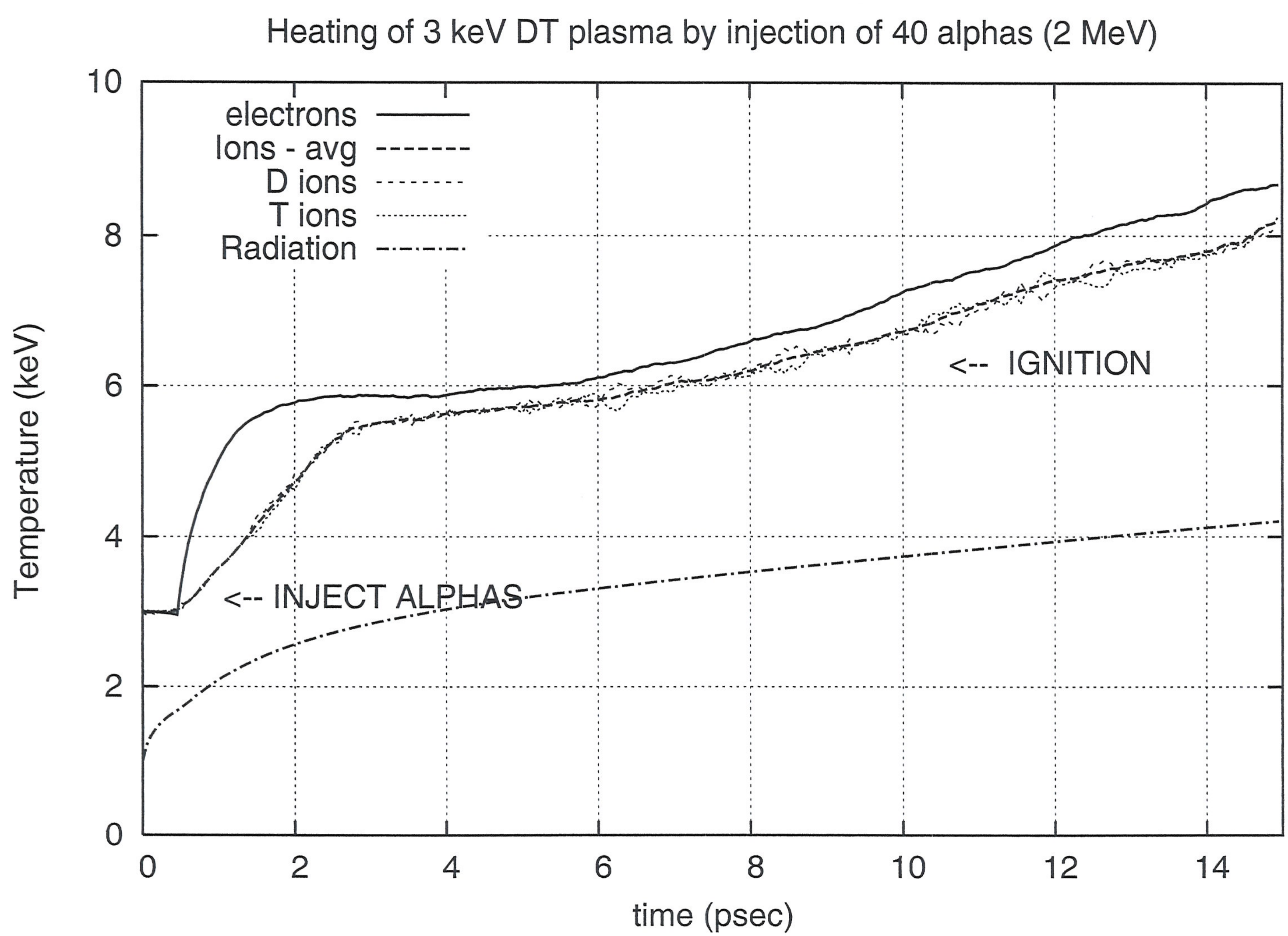
Here, inject 40 alphas ($E^0 = 2$ MeV) among 10,000 DT's

Find ignition about **3 psec** after the injection
Abundant "knock-on" DT ions

- The alphas obey periodic BC's, so they deposit

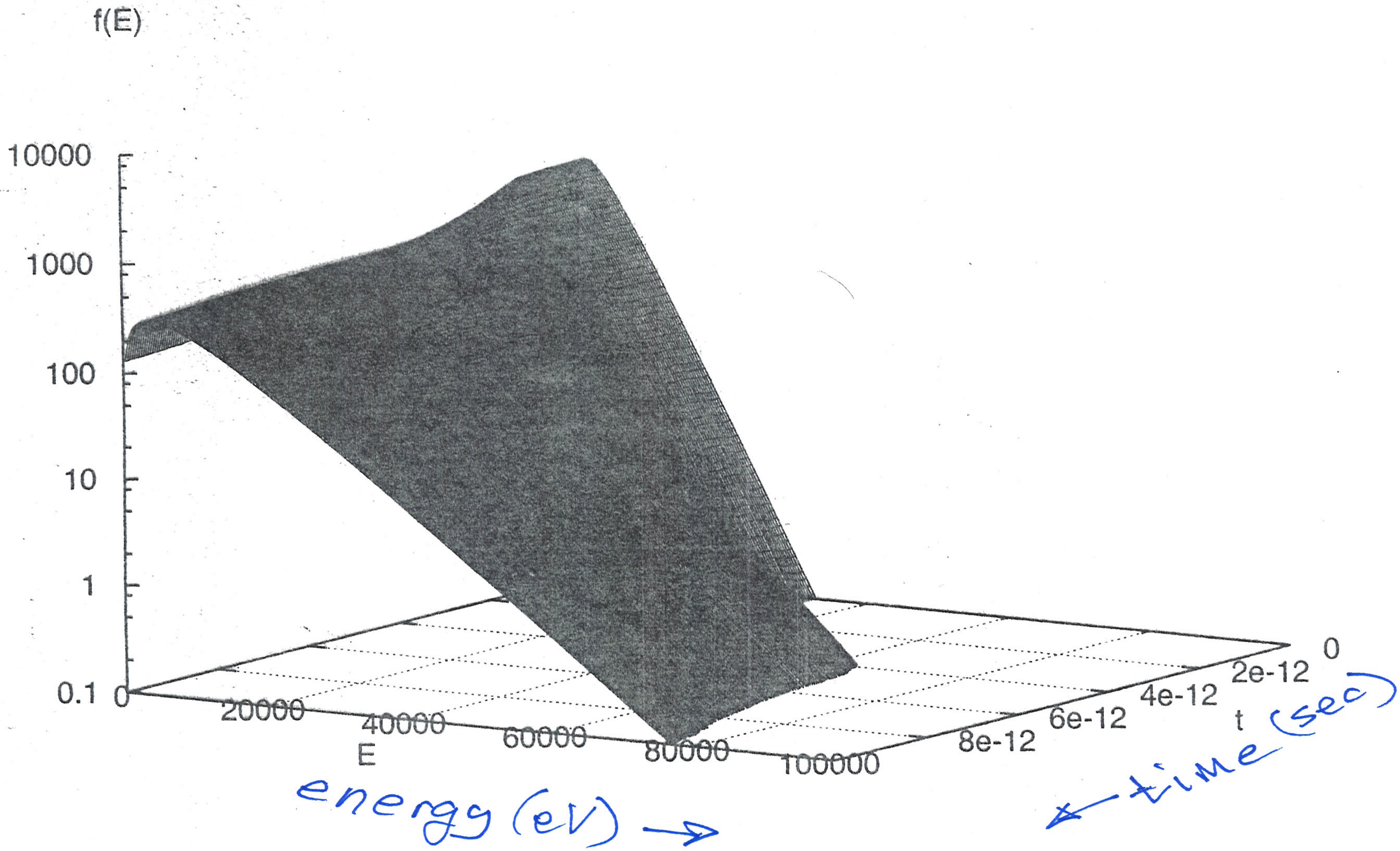
  310 MJ/gram or 80 Joules in 250 ngram

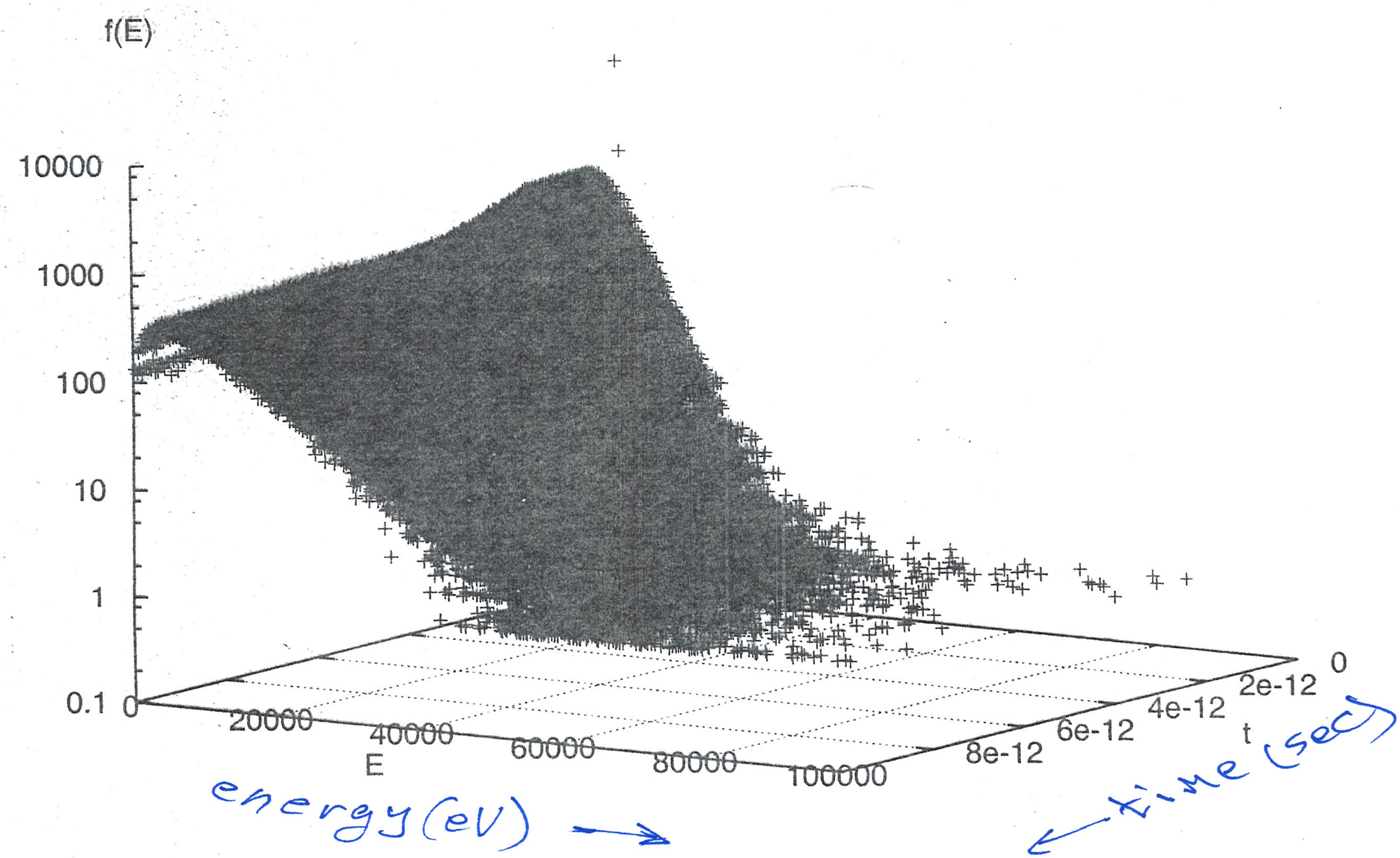
- High energy (MeV) electrons would probably couple more slowly



Heating of 3 keV DT plasma by injection of 40 alphas (2 MeV)
electrons
Ions - avg
D ions
T ions
Radiation
<-- INJECT ALPHAS
<-- IGNITION
Temperature (keV)
time (psec)
0
2
4
6
8
10
12
14

17


f(E)
10000
1000
100
10
1
0.1
0
20000
40000
60000
80000
100000
E
0
2e-12
4e-12
6e-12
8e-12
t
energy (eV) →
← time (sec)



f(E)
10000
1000
100
10
1
0.1
0
20000
40000
60000
80000
100000
E
0
2e-12
4e-12
6e-12
8e-12
t
energy (eV)
time (sec)

"*Barydiffusion*" ?

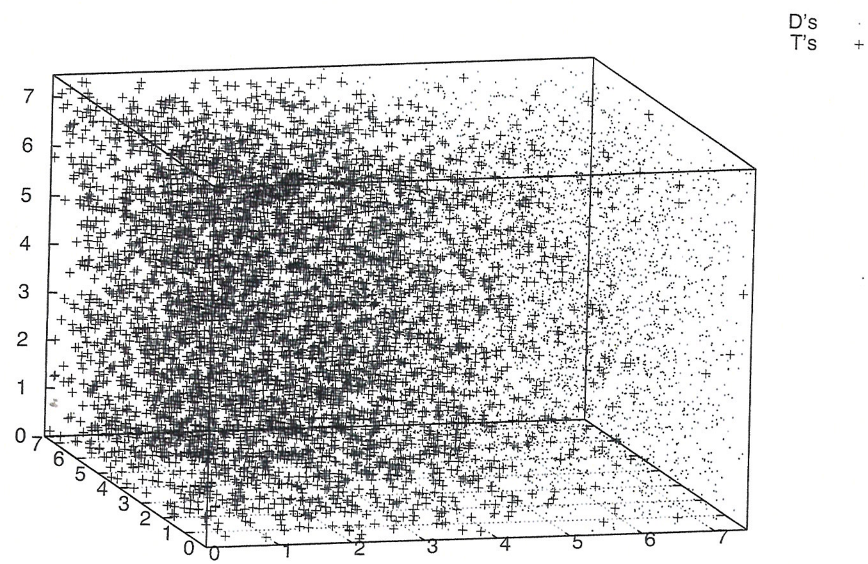
P. Amendt, LLNL

= partial segregation of D, T nuclei during target implosion

Do D, T diffuse and re-mix ? diffusion coefficient?

If most fusions involve E > 5 kT, does segregation matter ?

Do T_D, and T_T drift apart in segregated fuel ?



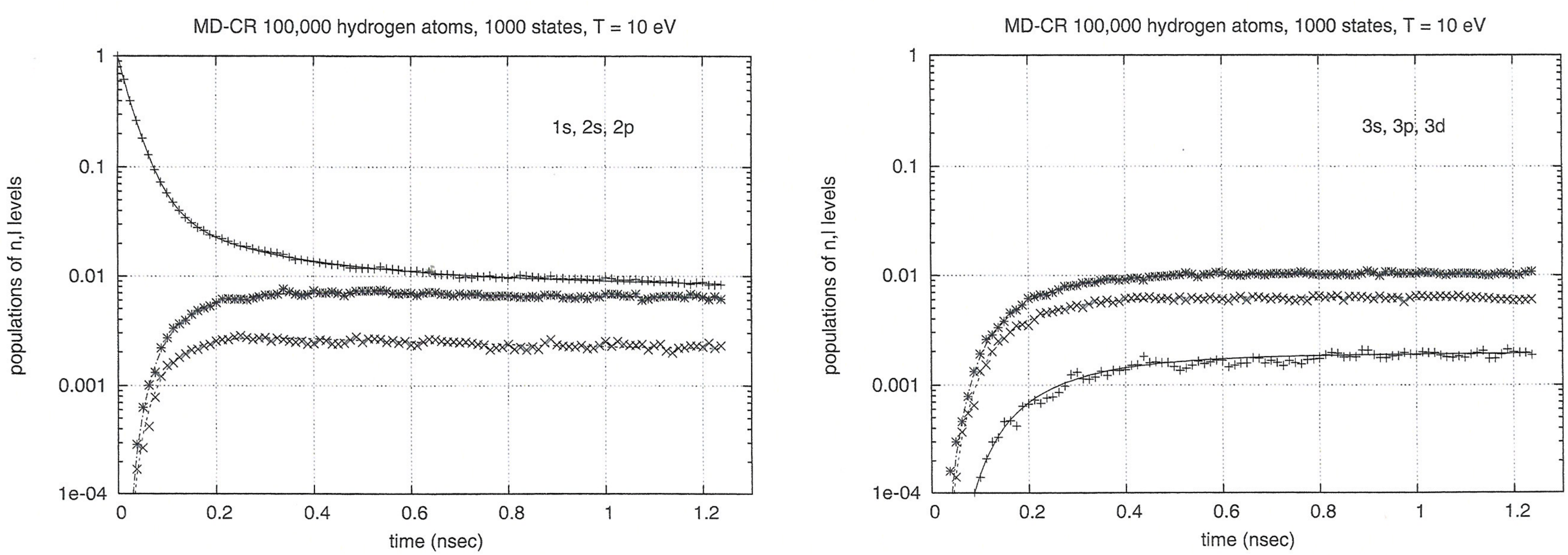
R. More, LBNL, and F. Wang (NAO, CAS)

Molecular Dynamics (atoms) plus Collisional-Radiative atomic model

First simple calculation:

Hydrogen in a fixed environment ($T_e = T_r$)
100,000 atoms with 1000 excited states (each)

The MD-CR correctly relaxes to equilibrium (LTE)



SUMMARY

- MD + electrons + radiation + fusion + alphas

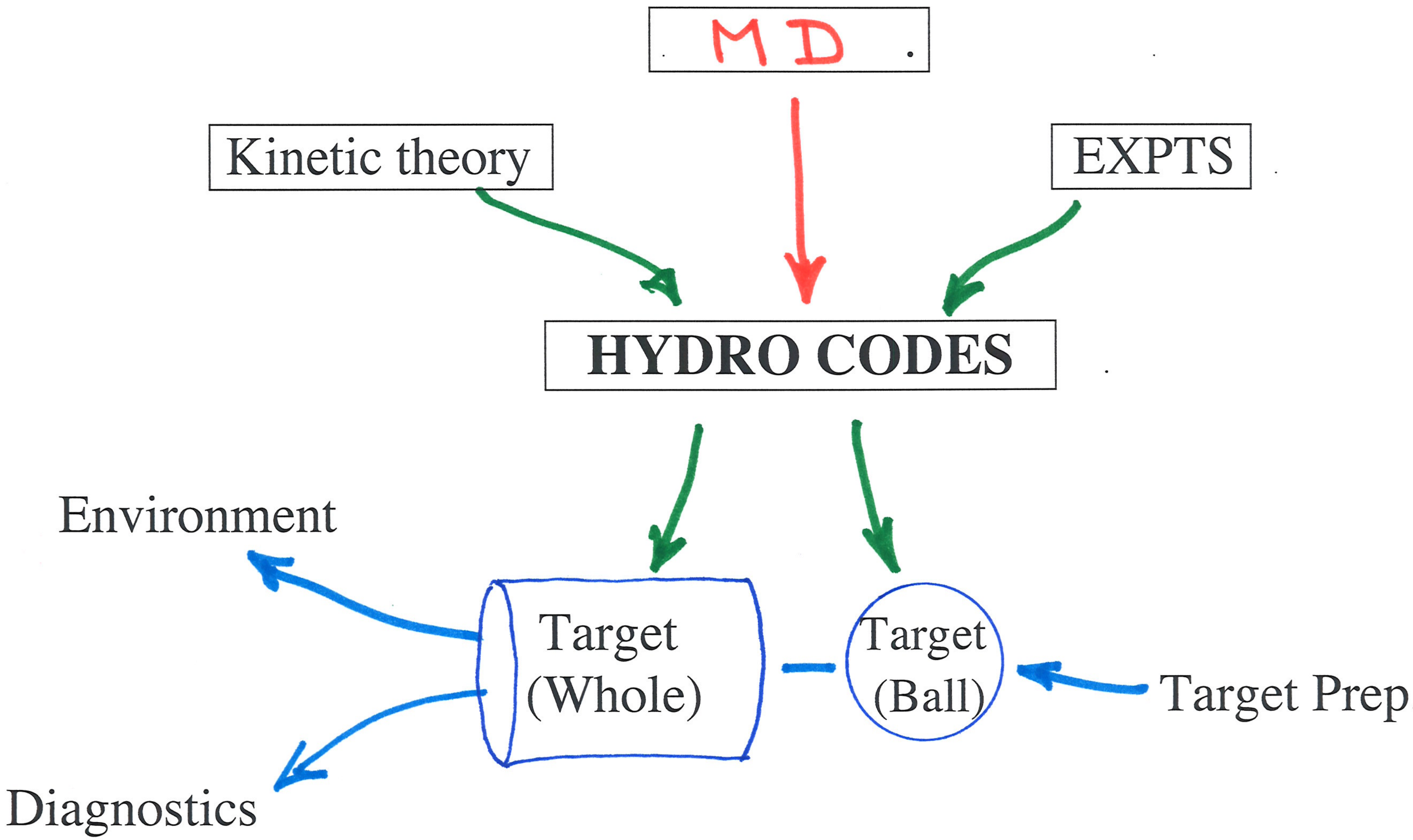
can give atomic-scale data about fusion

- MD can examine Fast-ion Fast-ignition

- Step 1 = MD for hard-spheres, point charges
  Step 2 = species mixtures (phase separation)
  Step 3 = MD for particles that react or get excited

  MD + CR model -- > line profiles
  MD + Chemisry -- > combustion, detonation

BIG PICTURE:



MD
Kinetic theory
EXPTS
HYDRO CODES
Environment
Target
(Whole)
Target
(Ball)
Target Prep.
Diagnostics

NOVEL FUSION ?

- o Spin-polarized DT fusion [PRL '83]
  Cross-section increases by ~ 50 %

- o Ion-quiver fusion [IFSA 2001]
  DT gas in focal spot of 10 PW laser

- o Muon catalyzed fusion