Dynamic Simulations Using Particle Models

2nd CEM Symposium, West Point, NY, April 3, 2018

DR. PAOLO ZANNETTI, QEP
PRESIDENT
THE ENVIROCOMP INSTITUTE WWW.ENVIROCOMP.ORG
ENVIROCOMP CONSULTING, INC. WWW.ENVIROCOMP.COM

Particle Modeling

- Particle modeling is the study of the dynamics behavior of solids and fluids in response to external forces
- Solids and fluids are modeled by a set of N fictitious, interactive “particles” that can represent atoms, or molecules, or aggregates of atoms and molecules
- A particle can vary from microscopic (a ion in a plasma) to macroscopic (a planet inside a galaxy)

Cont.

- Particles move at each time step Δt as a consequence of all forces acting on the particles
  - Interparticle forces
  - External forces (on a mesh)
- Three cases of interparticle forces
  1. Each particle motion is independent from the other N-1 particles
     - ➔ N computations every Δt
  2. Each particle motion is dependent upon interactions with the other N-1 particles
     - ➔ $\sim N^2$ computations every Δt
  3. Each particle interacts only with its immediate neighbors (Q particles), while the other particles (N-1-Q) only contribute as an external or long range force (on a mesh)
     - ➔ $\sim N \cdot Q$ computations every Δt

Greateast Advantages

- Most calculations are **grid-free**
- Powerful visualization ➔ diagnostics
- Many simulations would be almost impossible with traditional grid models
- Particle models can easily allow the addition of semi-random velocities to include the effects of physical components (e.g., turbulence) in a straightforward and relatively simple way (Monte Carlo generation of semi-random velocities)
- Suitable for parallel computing

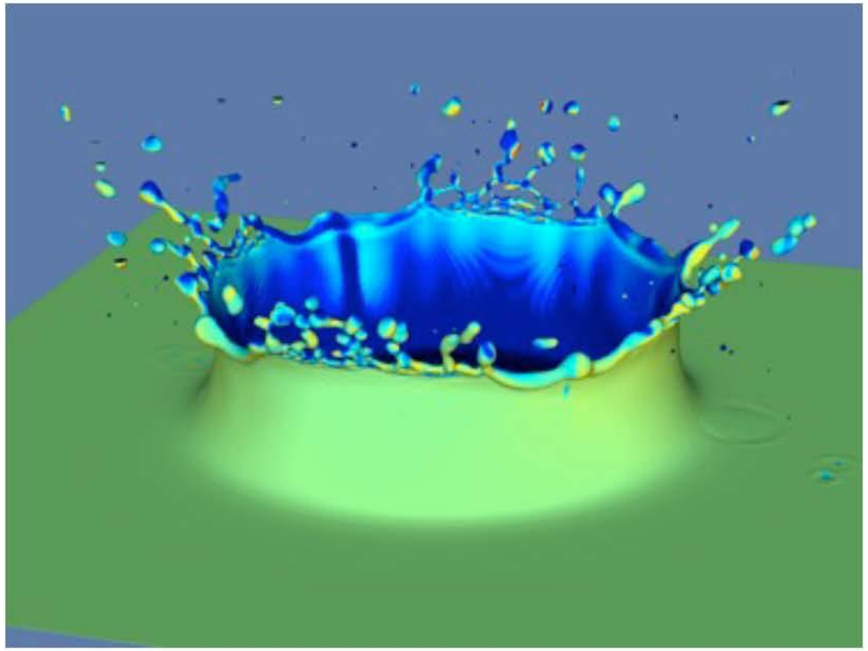
Mashfree Methods

Meshfree methods

The key idea is to provide accurate and stable numerical solutions to PDE's or integral equations with all kinds of possible boundary conditions

-using a set of arbitrarily distributed particles (or nodes) without any mesh.

Early work modified the internal structure of the grid-based methods to make them more adaptive, versatile and robust.

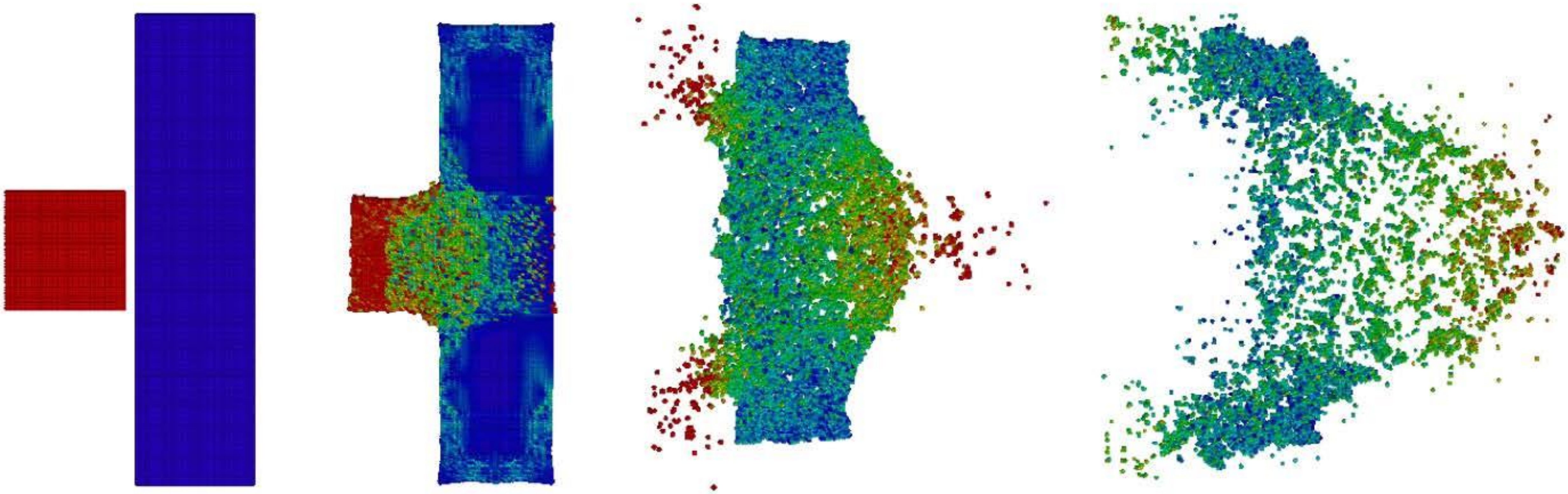


Droplet impact and splashing
Simulation of a splash performed by Pascal Ray.

Some Fields of Application

- Elastic strings
- Cavity flow
- Turbulence
- Liquid drops
- Crack development
- Fluid bubbles
- Relativistic motion
- Modeling fuzzy objects, such as fire, clouds, and water for the entertainment industry
- Semiconductors
- Astrophysics
- My field: **air pollution modeling in a turbulent atmosphere**

Collision of two bodies
(red = high velocity; blue = low velocity)



Fluid dynamics

- Sloshing
  - https://www.prometechsoftware.com/1-what-is-a-particle-method.html
- Pipe
  - https://www.prometechsoftware.com/1-what-is-a-particle-method.html
- Whirlpool
  - https://www.bing.com/videos/search?q=Double+Whirlpool+blender+2.66a+fluid+particles+simulation&view=detail&mid=3B8712FEECBF192726AF3B8712FEECBF192726AF&FORM=VIRE
- Interactive sloshing
  - https://www.bing.com/videos/search?q=Fluid+Particles-+Real-time+particle-based+3D+fluid+simulation&view=detail&mid=1D91BF6FED1A2B9FFCF51D91BF6FED1A2B9FFCF5&FORM=VIRE

Electron Flow in Semiconductors Initial Conditions

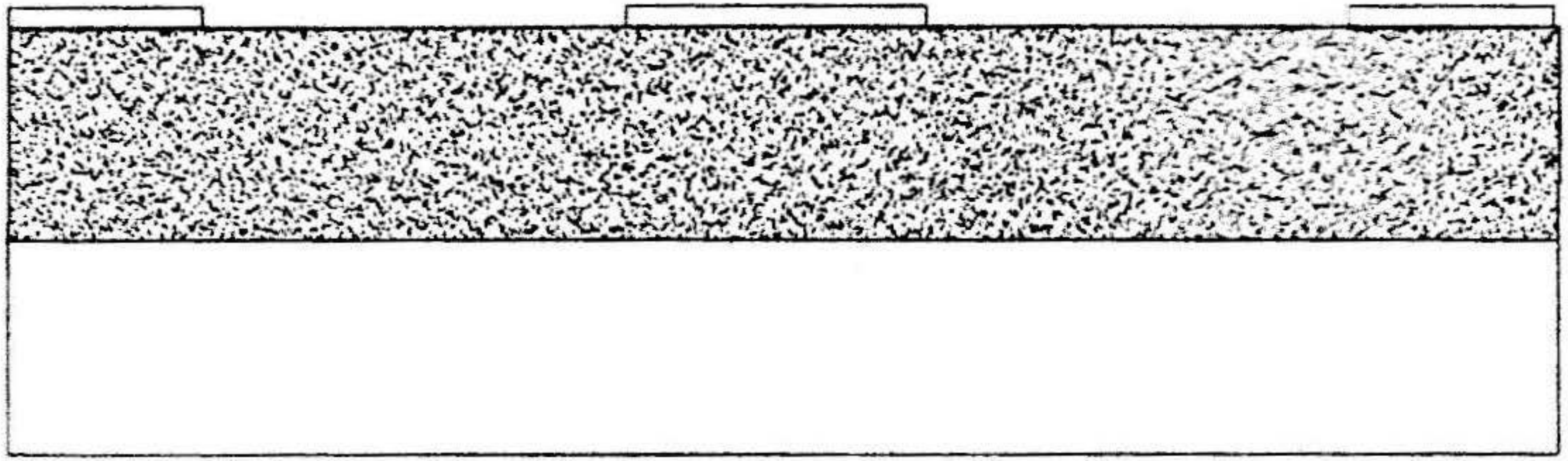


Figure 10-13 The charge-neutral initial condition. The simulated electrons that are shown are all in Band I at 300 K. The voltages on all electrodes are zero. (*Courtesy of S. J. Beard.*)

Steady-state Conditions

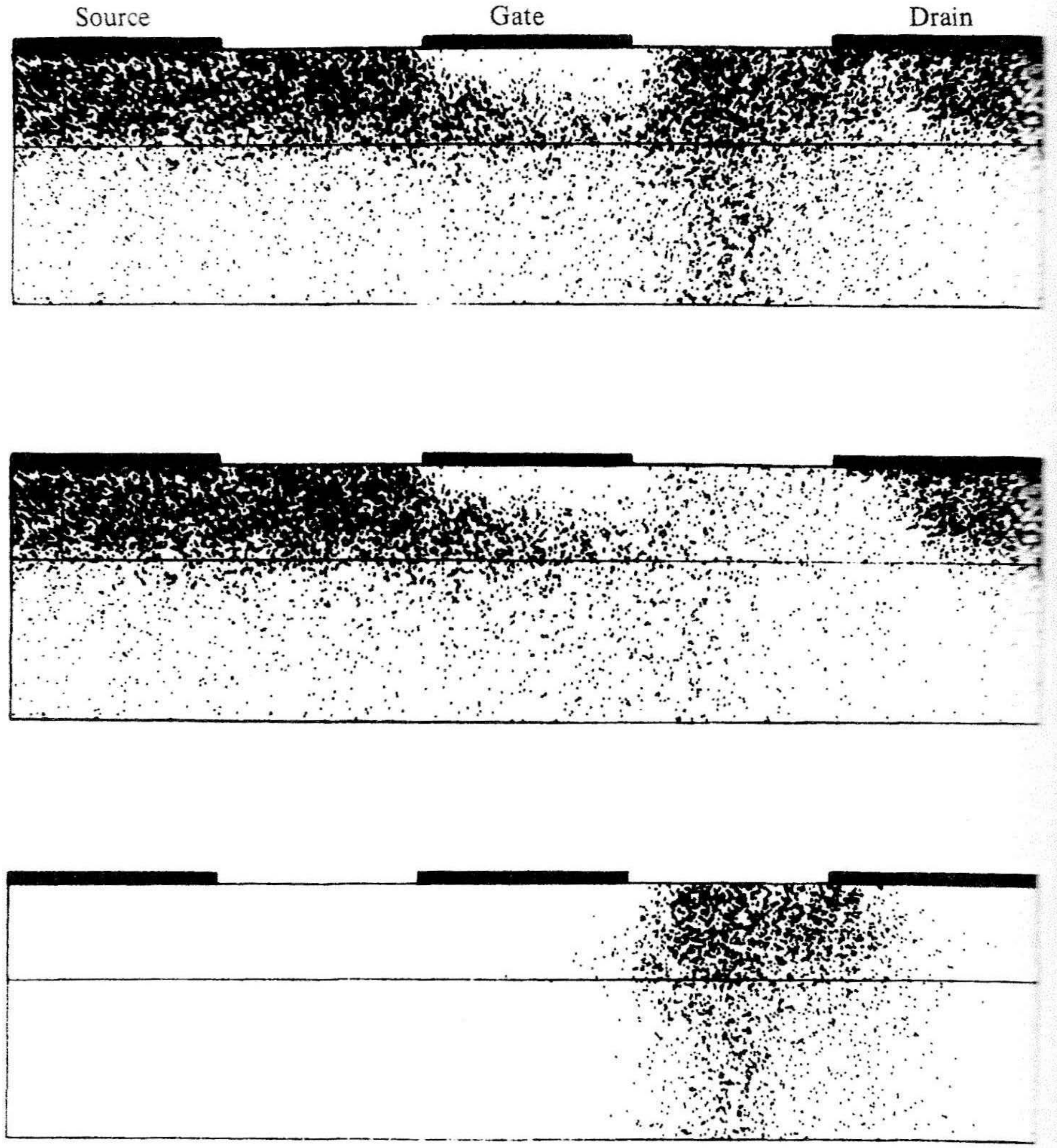
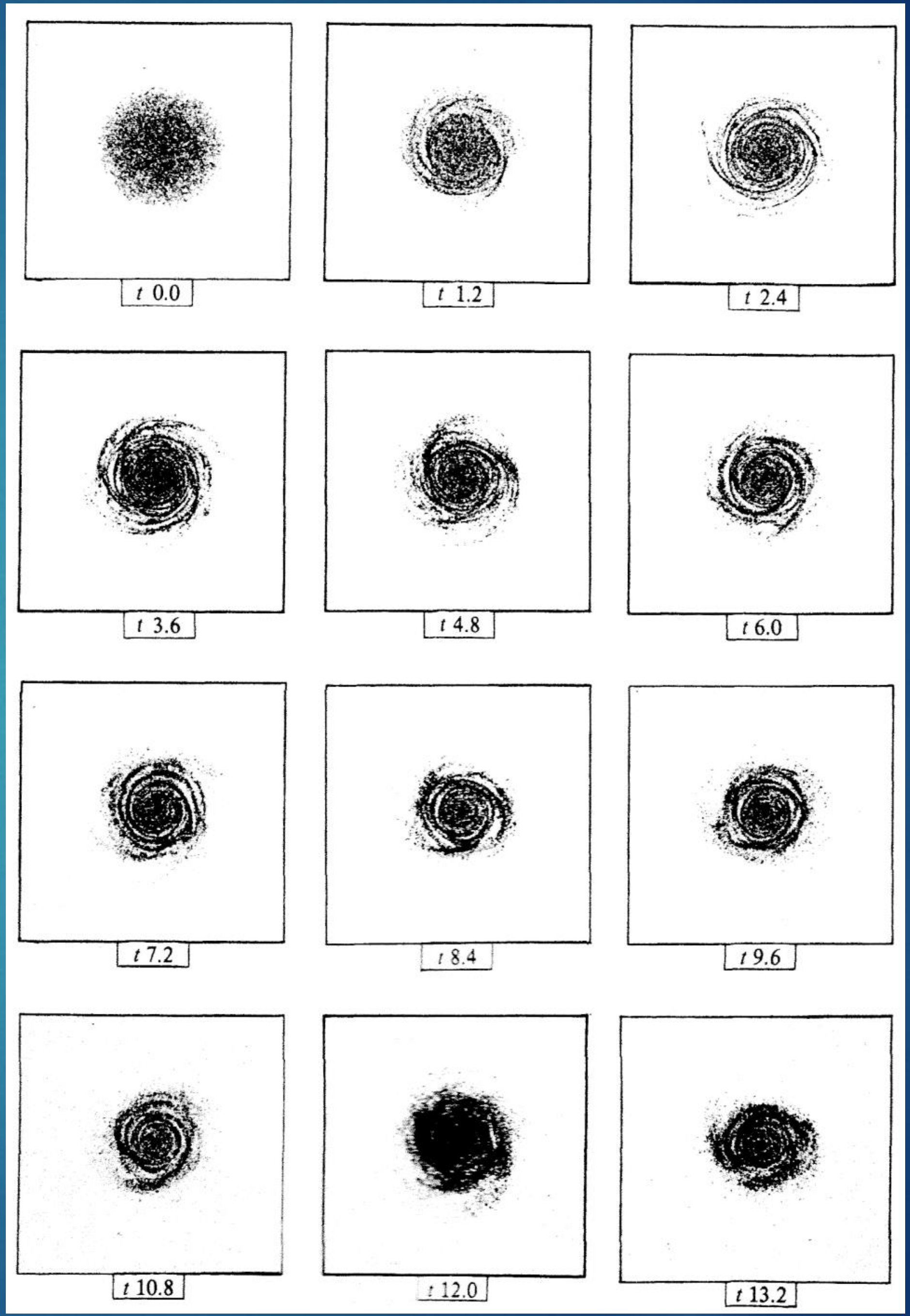


Figure 10-17 The distribution of electrons at the normal operating point ($V_D = 3.0$ V, $V_G = -1.02$ V). *Top*, all electrons; *centre*, Band I electrons; *bottom*, Band II electrons. Note the Band II electrons in the high-field region between gate and drain and the substantial current flowing in the substrate. The epitaxial/substrate boundary is shown by a horizontal line. (*From Hockney, Warriner, and Reiser, 1974; courtesy of Electronics Letters,* © *Institution of Electrical Engineers.*)

Astrophysics

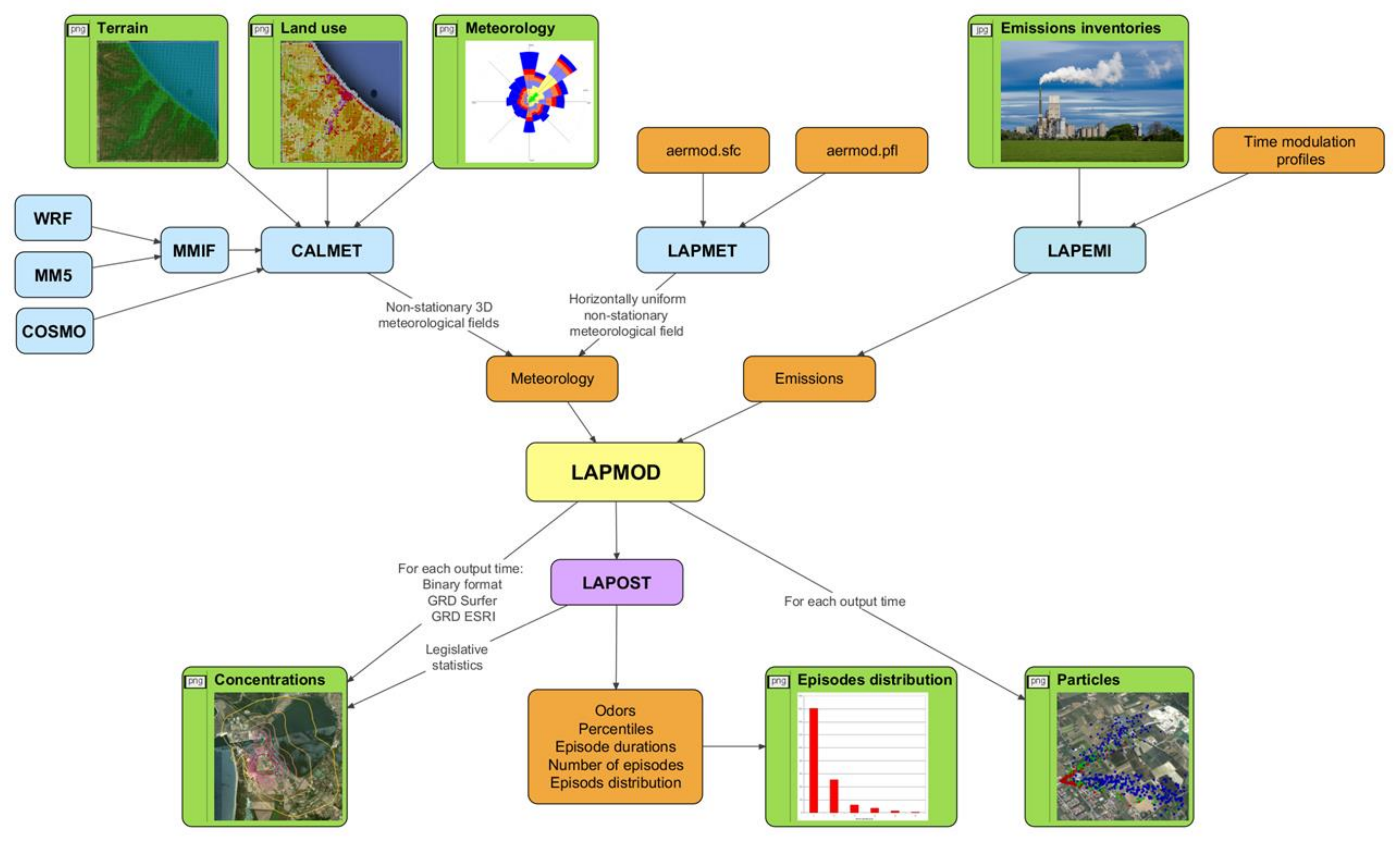
More info on cosmological simulations: http://phys.huji.ac.il/~joaw/winterschool/teyssier_lecture_1.pdf



Air Pollution Modeling

- "Natural", intuitive way of simulating air pollution
  - A "particle" is a tracer point representing a mass of emitted pollutant
  - Particles moves according to a 3D wind vector plus a turbulent, semi-random velocity generated by Monte Carlo methods
  - No interparticle forces!
  - Example:
    - http://www.envirocomp.com/caps/projects/monsanto/v1.html

LAPMOD



png Terrain
png Land use
png Meteorology
jpg Emissions inventories
aermod.sfc
aermod.pfl
Time modulation profiles
WRF
MM5
COSMO
MMIF
CALMET
LAPMET
LAPEMI
Non-stationary 3D meteorological fields
Horizontally uniform non-stationary meteorological field
Meteorology
Emissions
LAPMOD
For each output time: Binary format GRD Surfer GRD ESRI
LAPOST
For each output time
Legislative statistics
png Concentrations
Odors
Percentiles
Episode durations
Number of episodes
Episods distribution
png Episodes distribution
png Particles

LAPMOD info

- free download: https://www.enviroware.com/lapmod/
- Paper: http://www.envirocomp.com/zcv/JA.27.pdf

END

- Thank you!
- zannetti@envirocomp.com