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CPU and GPU-based Numerical Simulations of Combustion Processes

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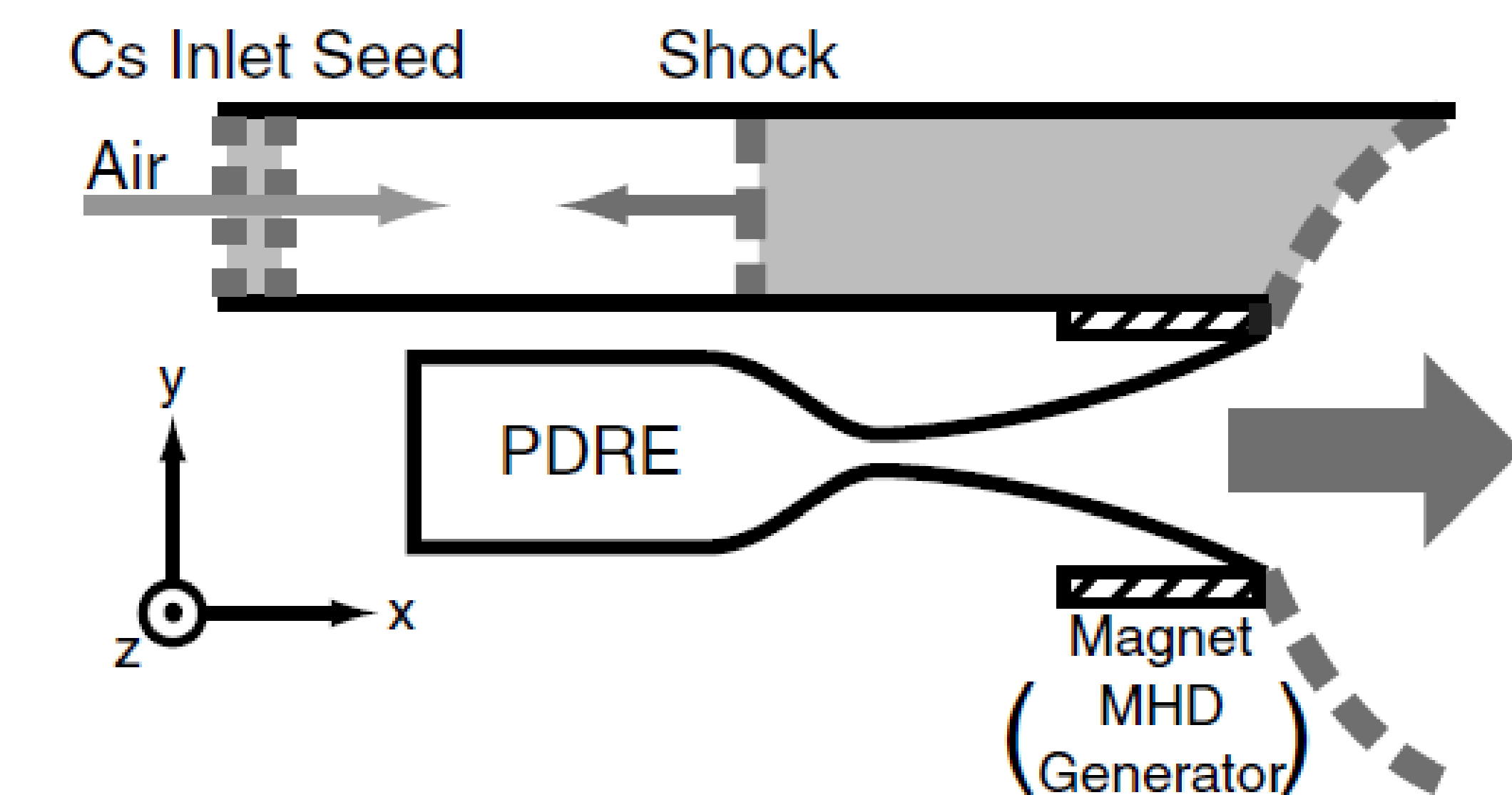
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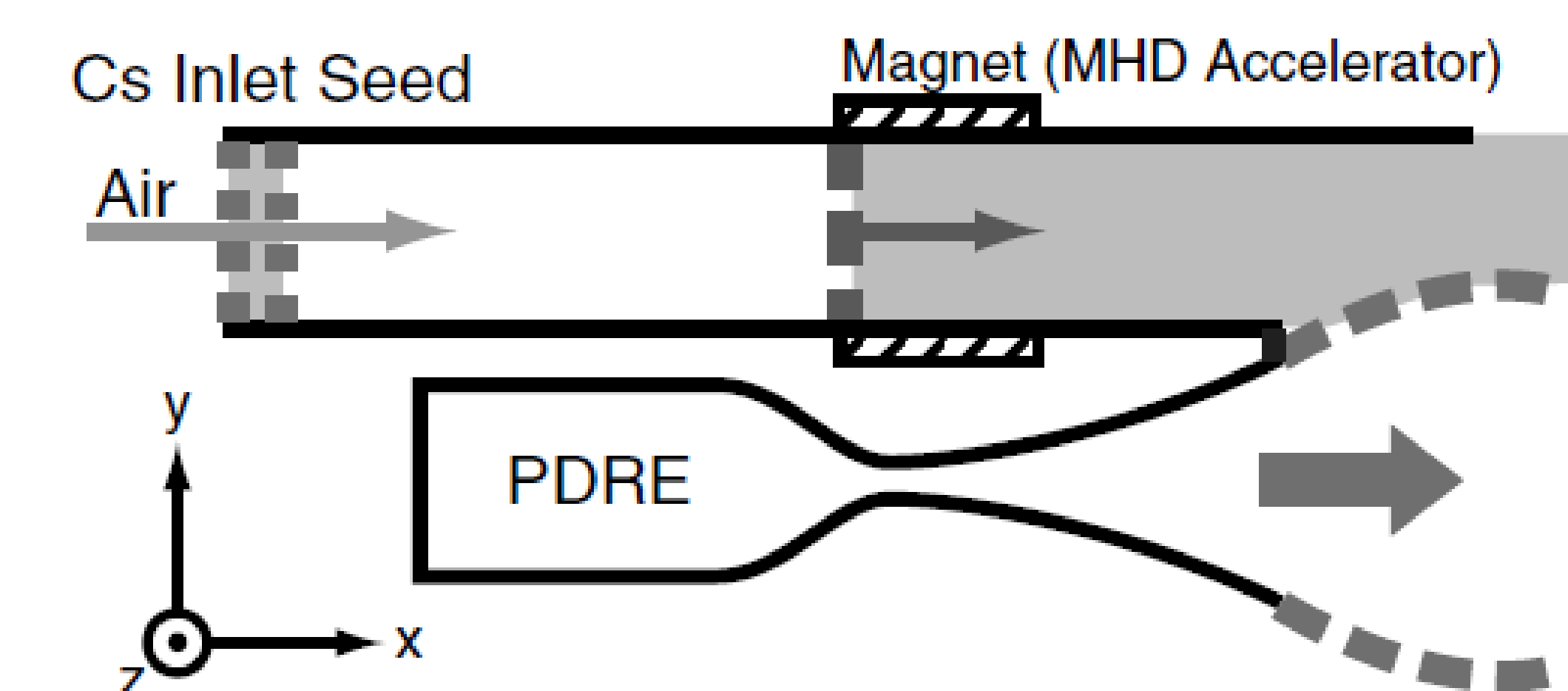
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Magnetohydrodynamic Augmentation of the Pulse Detonation Rocket Engines

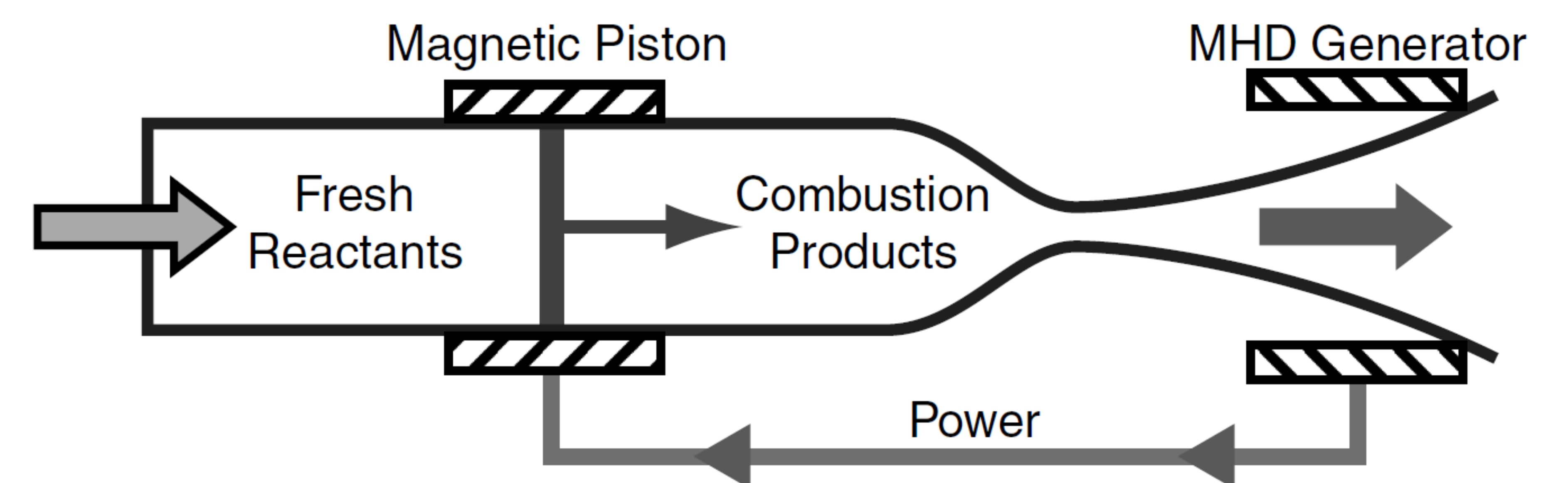
- Pulse Detonation Rocket-Induced MHD Ejector (PDRIME)
 - Energy extract from exhaust flow by MHD generator
 - Seeded air stream acceleration by MHD accelerator for thrust enhancement and control
- Alternative concept: Magnetic piston
 - During PDE blowdown process, MHD extracts energy and applies to chamber gas via a magnetic piston or MHD generator to maintain constant chamber pressure and temperature



a)



b)



Simplified Physical Models

- Euler fluid transport with WENO

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x + \mathbf{G}(\mathbf{U})_y = \mathbf{S}(\mathbf{U}) + \mathbf{M}(\mathbf{U})$$

- One-step kinetics (ionization of cesium)



$$\begin{pmatrix} \dot{\Omega}_{\text{Cs}} \\ \dot{\Omega}_{\text{Cs}^+} \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} [\text{Cs}] \\ [\text{Cs}^+] \end{pmatrix} = \begin{pmatrix} -k_f[\text{Cs}][\text{M}] + k_r[\text{Cs}^+][\text{M}][\text{e}^-] \\ k_f[\text{Cs}][\text{M}] - k_r[\text{Cs}^+][\text{M}][\text{e}^-] \end{pmatrix}$$

- Fixed electromagnetic field line

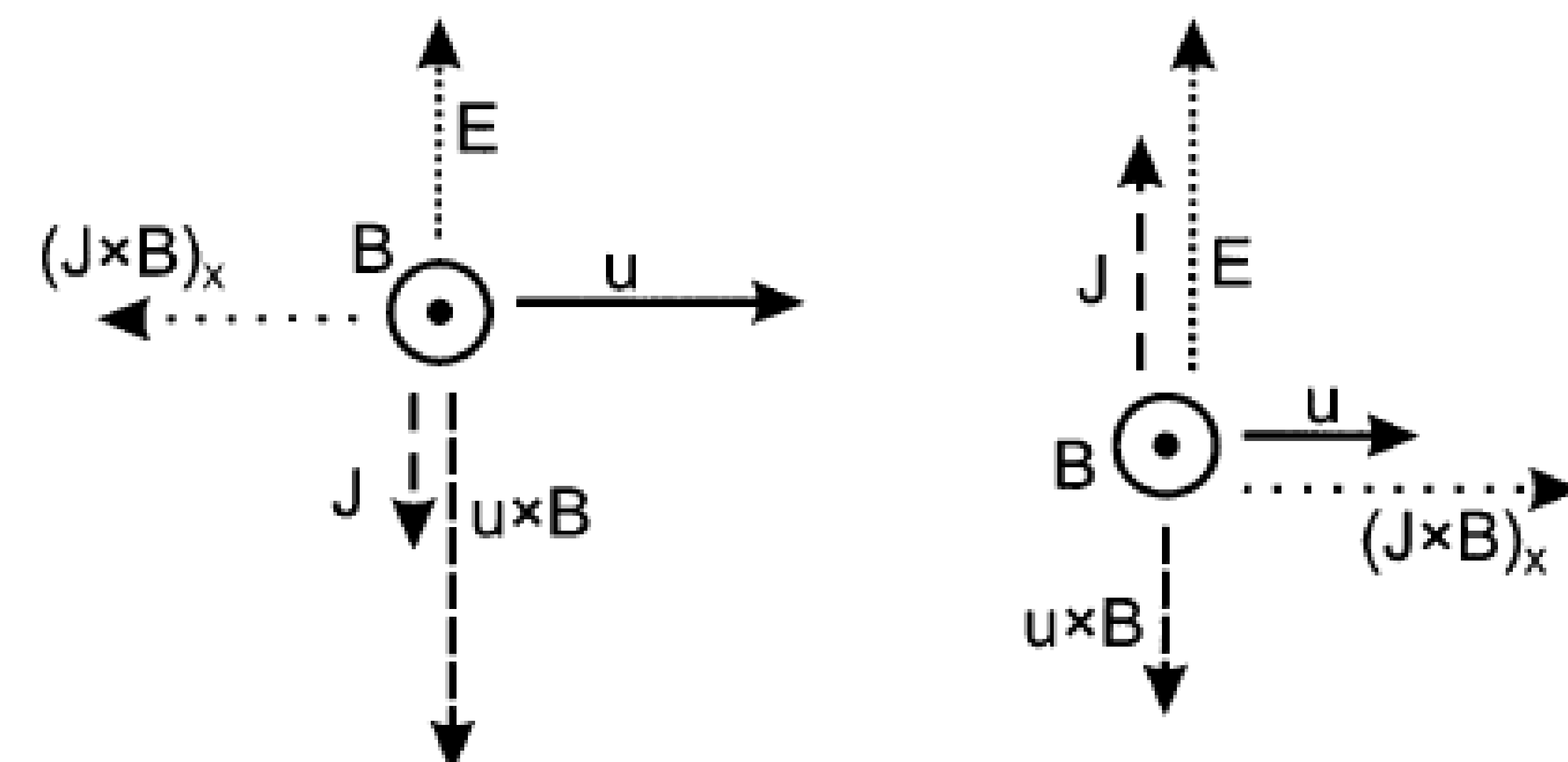
- Lorentz force

$$\mathbf{F}_L = \mathbf{J} \times \mathbf{B}$$

$$\mathbf{J} = \sigma(\mathbf{E} + \mathbf{u} \times \mathbf{B})$$

- MHD energy source term

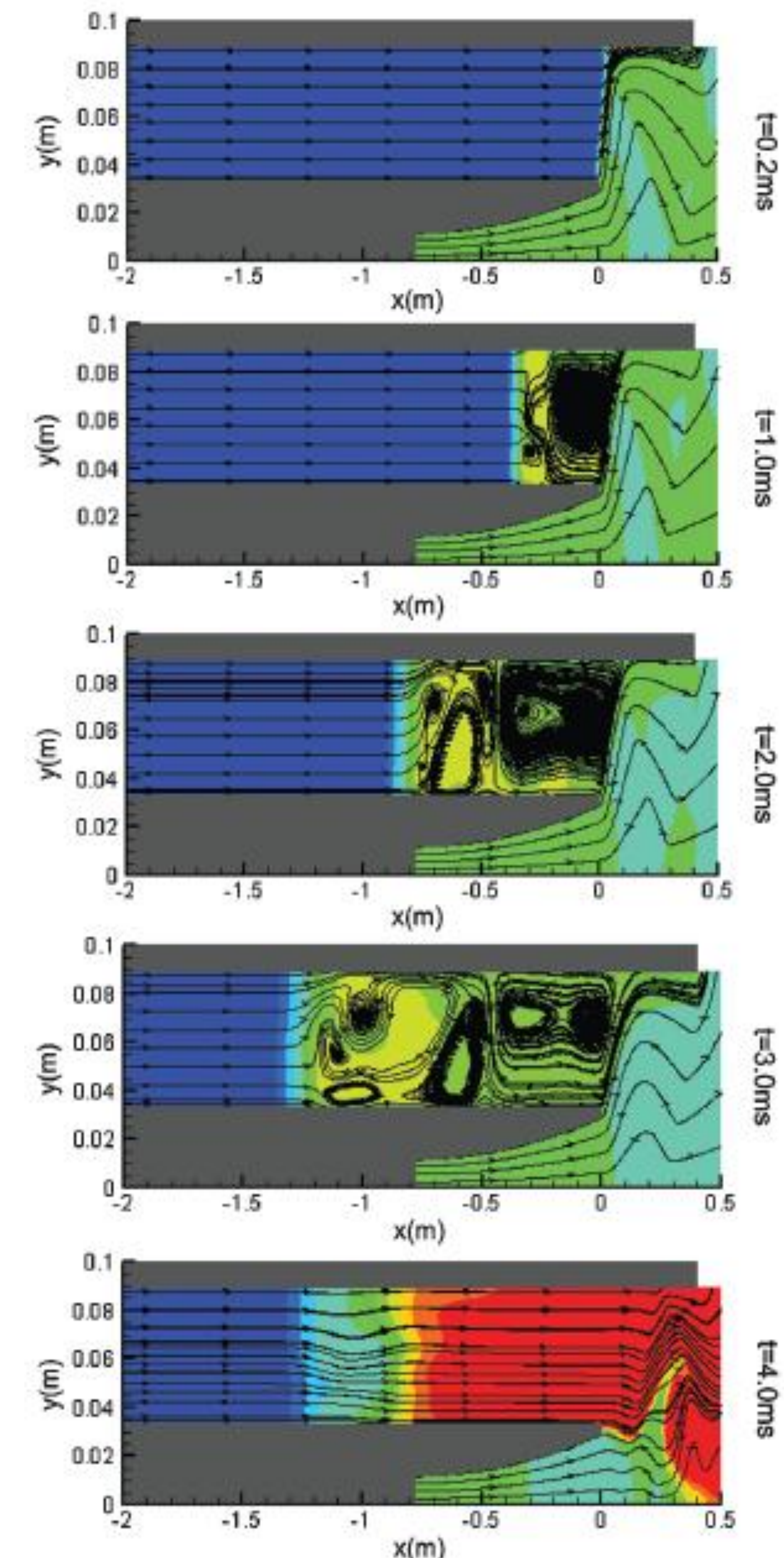
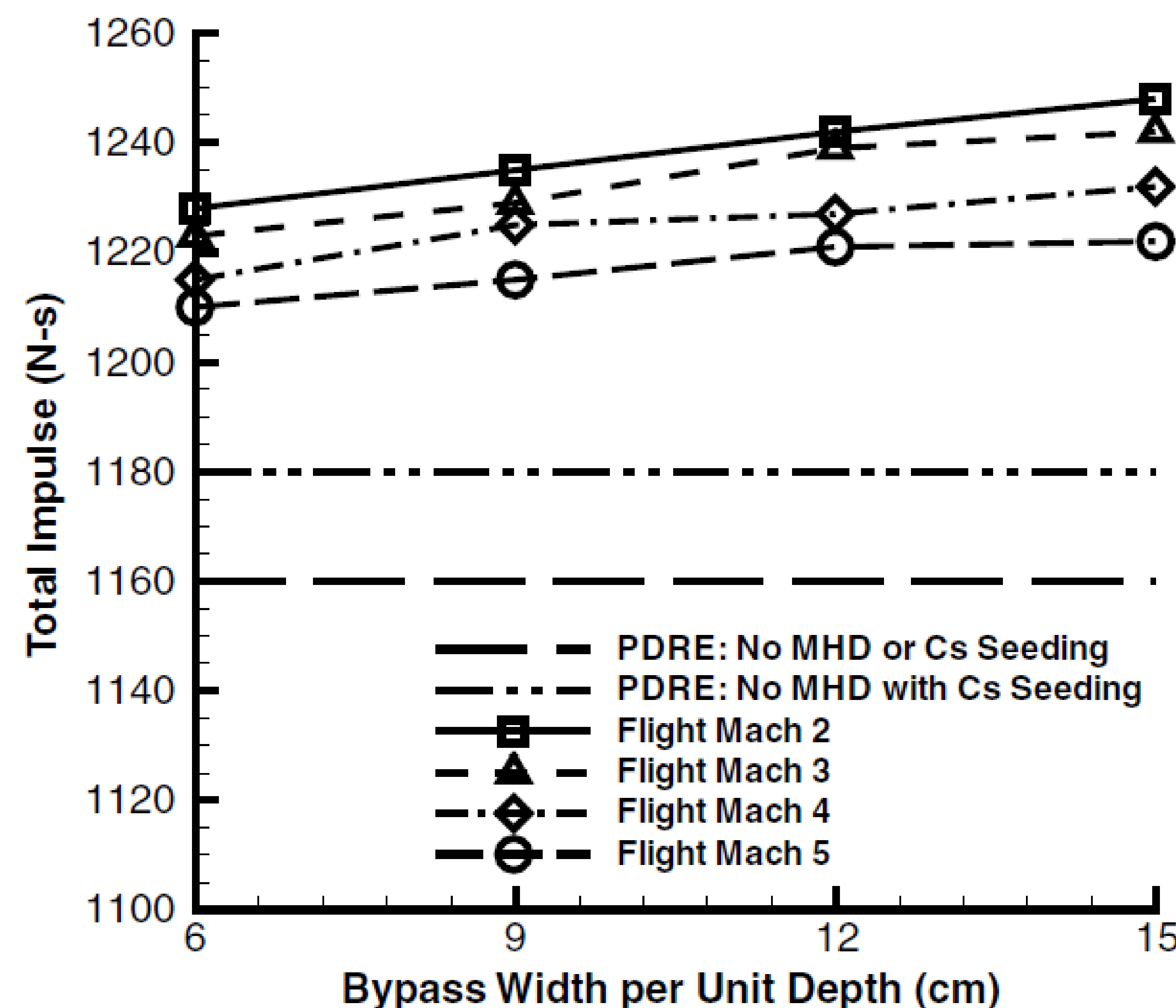
$$\mathbf{J} \cdot \mathbf{E} = \frac{\mathbf{J}^2}{\sigma} + \mathbf{u} \cdot (\mathbf{J} \times \mathbf{B})$$



MHD Generator (Nozzle) MHD Accelerator (Bypass tube)

Numerical Simulations of PDRIME

- Temperature contour of a PDRIME operating at 25 km, chamber temperature of 3000K and flight Mach number of 9
- Total impulse per cycle at 30 km and bypass area per unit length. Initial chamber of 3000 K and bypass length is 6 m. The chamber is seeded with 0.5% Cs and the bypass tube is seeded with 0.1% Cs (by moles).



Detailed Physical Models

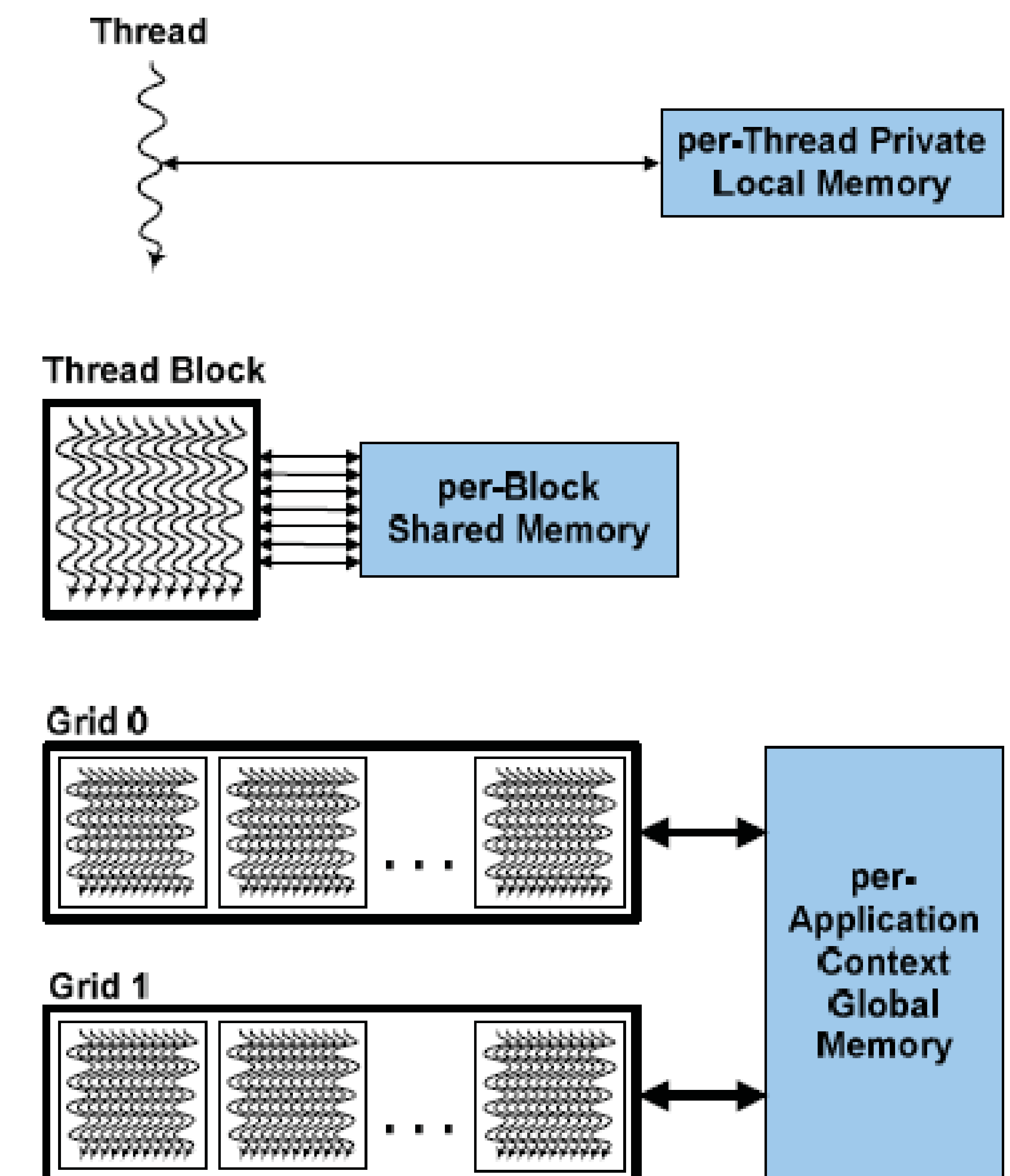
- Euler fluid transport with high-order shock capturing schemes: MP5, WENO, etc. in thermochemical nonequilibrium (2T model).
- Complex chemical kinetics for combustion processes
- Collisional-Radiative kinetics for electronic excitation and ionization.
- Electromagnetic field coupling via ideal and resistive MHD

$$\frac{dQ}{dt} + \frac{1}{V} \oint_S F_n dS = \dot{\Omega},$$

$$Q = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_n \\ \rho u \\ \rho v \\ \rho w \\ B_x \\ B_y \\ B_z \\ E \\ \rho \hat{s}_e \end{pmatrix}, \quad F_n = \begin{pmatrix} \rho_1 v_n \\ \vdots \\ \rho_n v_n \\ \rho u v_n + n_x p_o - B_x B_n / \mu_o \\ \rho v v_n + n_y p_o - B_y B_n / \mu_o \\ \rho w v_n + n_z p_o - B_z B_n / \mu_o \\ v_n B_x - u B_n \\ v_n B_y - v B_n \\ v_n B_z - w B_n \\ v_n (E + p_o) - B_n (\vec{v} \cdot \vec{B}) / \mu_o \\ v_n S_e \end{pmatrix} \quad A = \frac{\partial F}{\partial Q} = \begin{pmatrix} u(1-y_1) & \dots & -u y_1 & y_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -u y_n & \dots & u(1-y_n) & y_n & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ P_{\rho_1} - u^2 & \dots & P_{\rho_n} - u^2 & P_{m_x} + 2u & P_{m_y} & P_{m_z} & P_{B_x} - \frac{B_x}{\mu_o} & P_{B_y} + \frac{B_y}{\mu_o} & P_{B_z} + \frac{B_z}{\mu_o} & P_E & P_{S_e} \\ -uv & \dots & -uv & v & u & 0 & -\frac{B_y}{\mu_o} & -\frac{B_z}{\mu_o} & 0 & 0 & 0 \\ -uw & \dots & -uw & w & 0 & u & -\frac{B_x}{\mu_o} & 0 & -\frac{B_z}{\mu_o} & 0 & 0 \\ \frac{v B_x - u B_y}{\rho} & \dots & \frac{v B_x - u B_y}{\rho} & \frac{B_y}{\rho} & -\frac{B_x}{\rho} & 0 & -v & u & 0 & 0 & 0 \\ \frac{w B_x - u B_z}{\rho} & \dots & \frac{w B_x - u B_z}{\rho} & \frac{B_z}{\rho} & 0 & -\frac{B_x}{\rho} & -w & 0 & u & 0 & 0 \\ \leftarrow \partial f_E / \partial Q \rightarrow \\ -\frac{u}{\rho} S_e & \dots & -\frac{u}{\rho} S_e & \frac{1}{\rho} S_e & 0 & 0 & 0 & 0 & 0 & 0 & u \end{pmatrix}$$

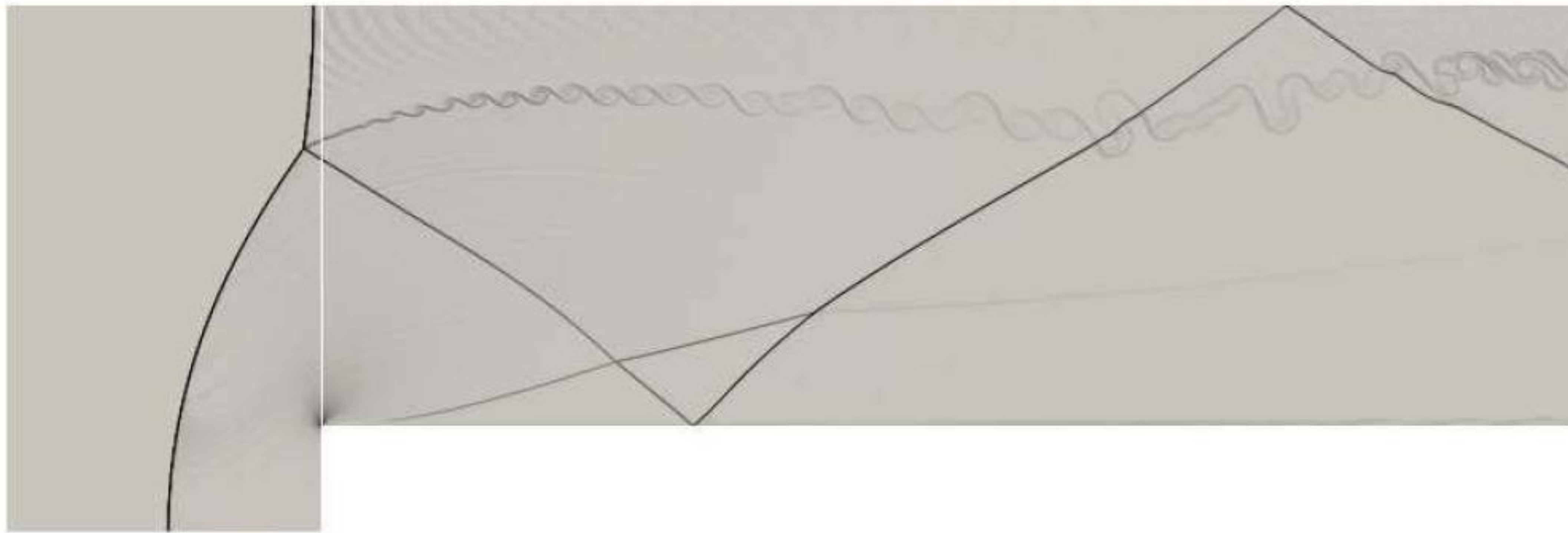
HPC Capability: Graphic Processing Units

- Graphic Processing Units
 - Graphic processing units containing a massive amount of processing cores designed for graphic rendering
 - GPU is faster than CPU on SIMD execution model.
 - GPGPU programming is very identical to traditional C/C++ (or Fortran). Object-Oriented features are available in CUDA.
 - GPU is much cheaper than CPU. The performance/dollar ratio for GPU is at least 16 times higher than CPU.
- Hoffman 2 ARK gpu queue configuration
 - 6 computing nodes (3 Tesla Fermi M2070 GPUs/node)
 - Supports MPI, CUDA, OpenCL, etc.

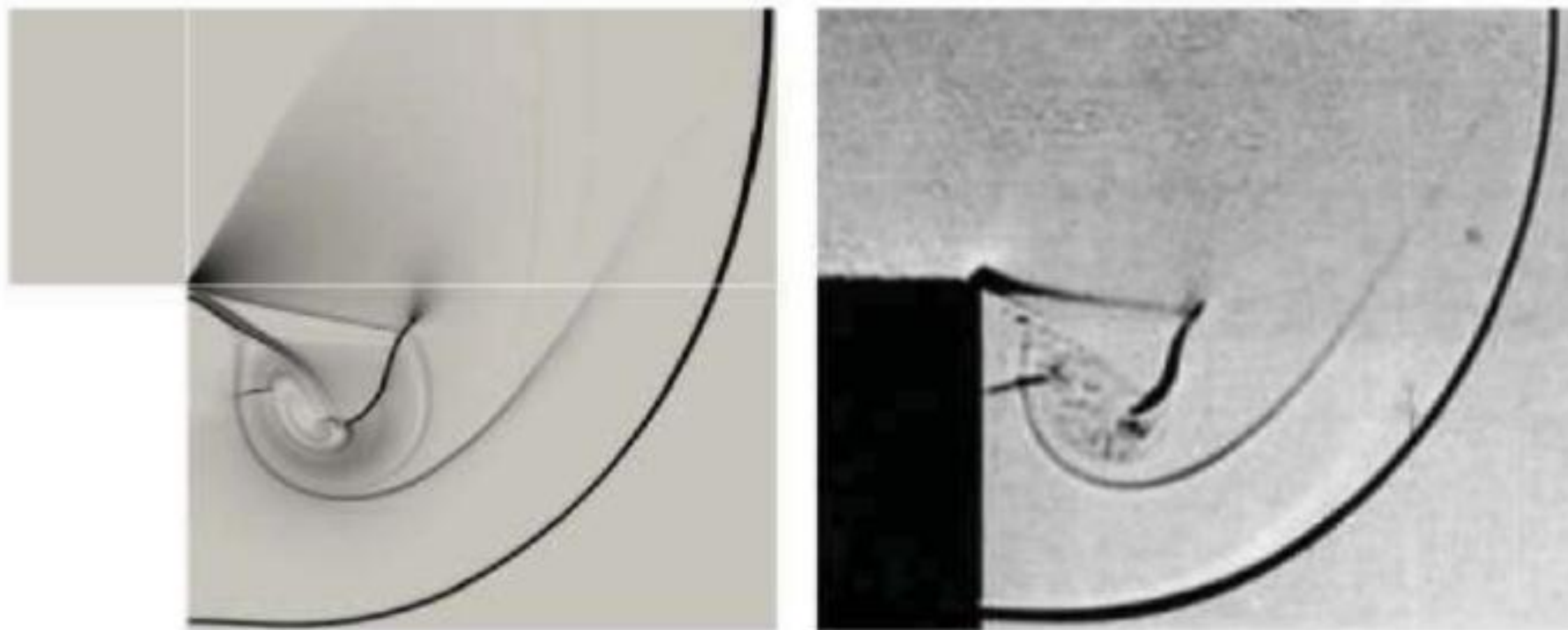


High-order Simulations of Fluid Flows

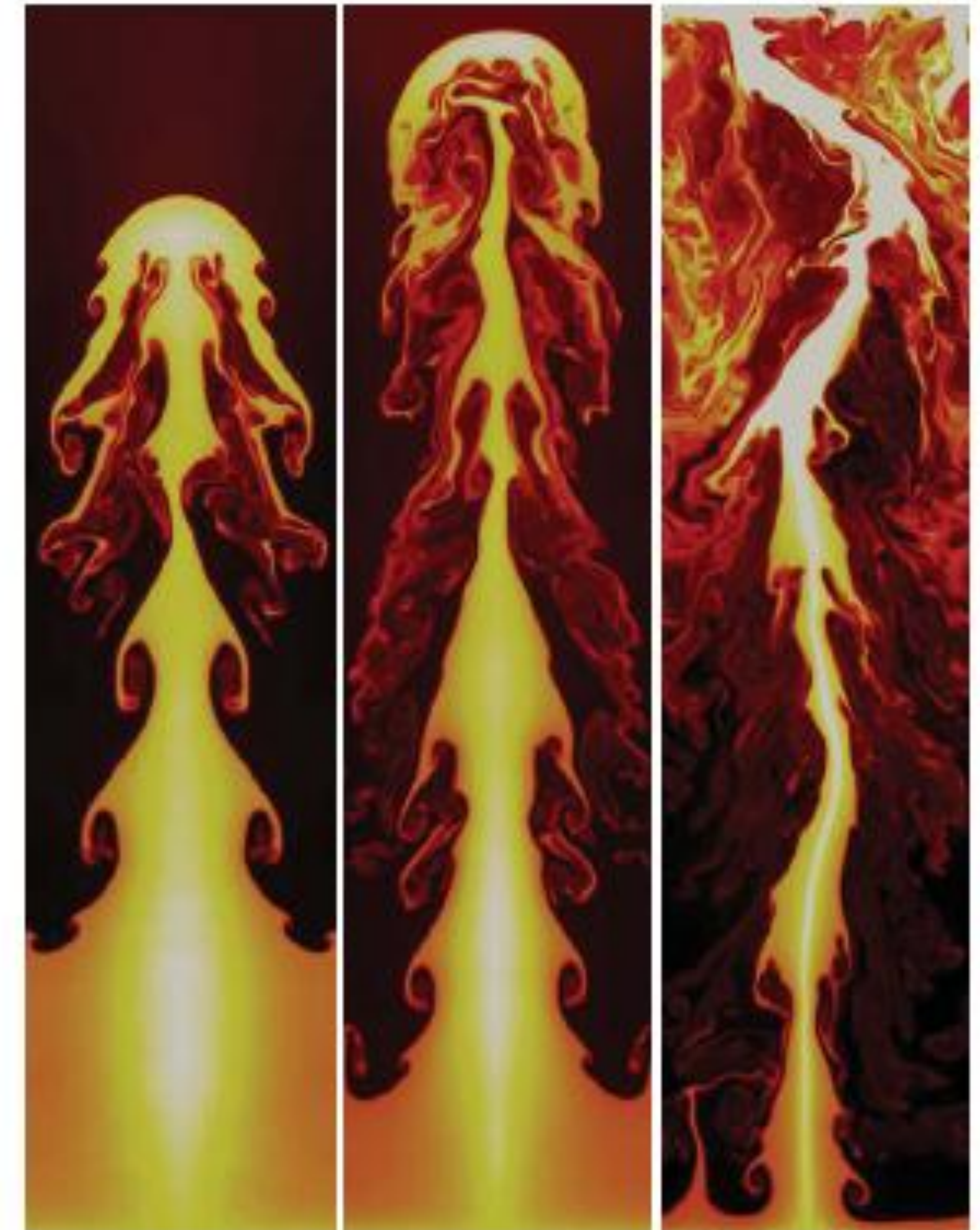
- Standard test cases for ideal gas flow:



Forward step problem (800,000 cells)



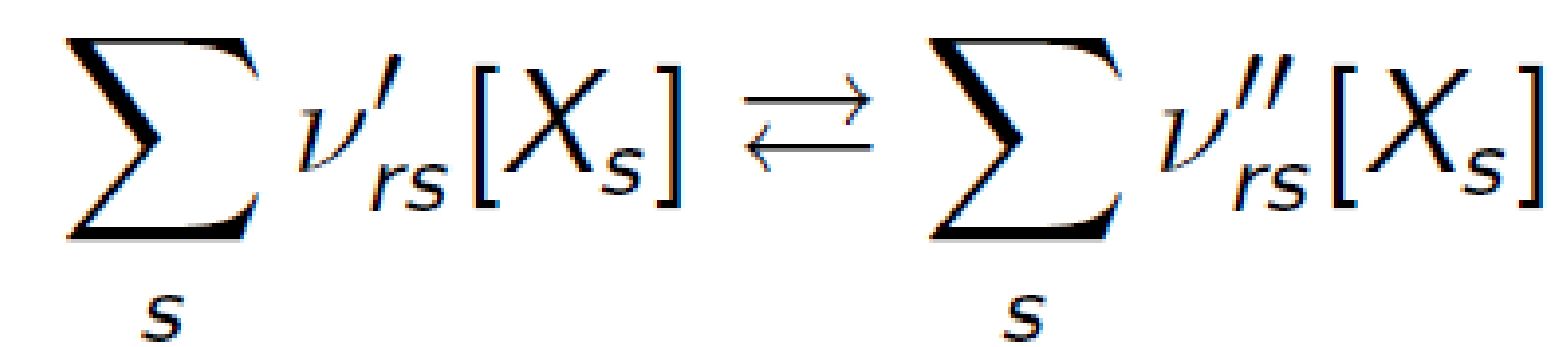
Backward step problem (27,000 cells)



Rayleigh-Taylor instabilities problem (1.6 Mcells)

Complex Kinetics

- Chemical kinetics



$$\dot{\omega}_s = \sum_r \nu_{rs} K_{fr} \prod_s [X_s]^{\nu'_{rs}} - \sum_r \nu_{rs} K_{br} \prod_s [X_s]^{\nu''_{rs}}$$

$$\nu_{rs} = \nu''_{rs} - \nu'_{rs}$$

- Collisional-Radiative (CR) Kinetics

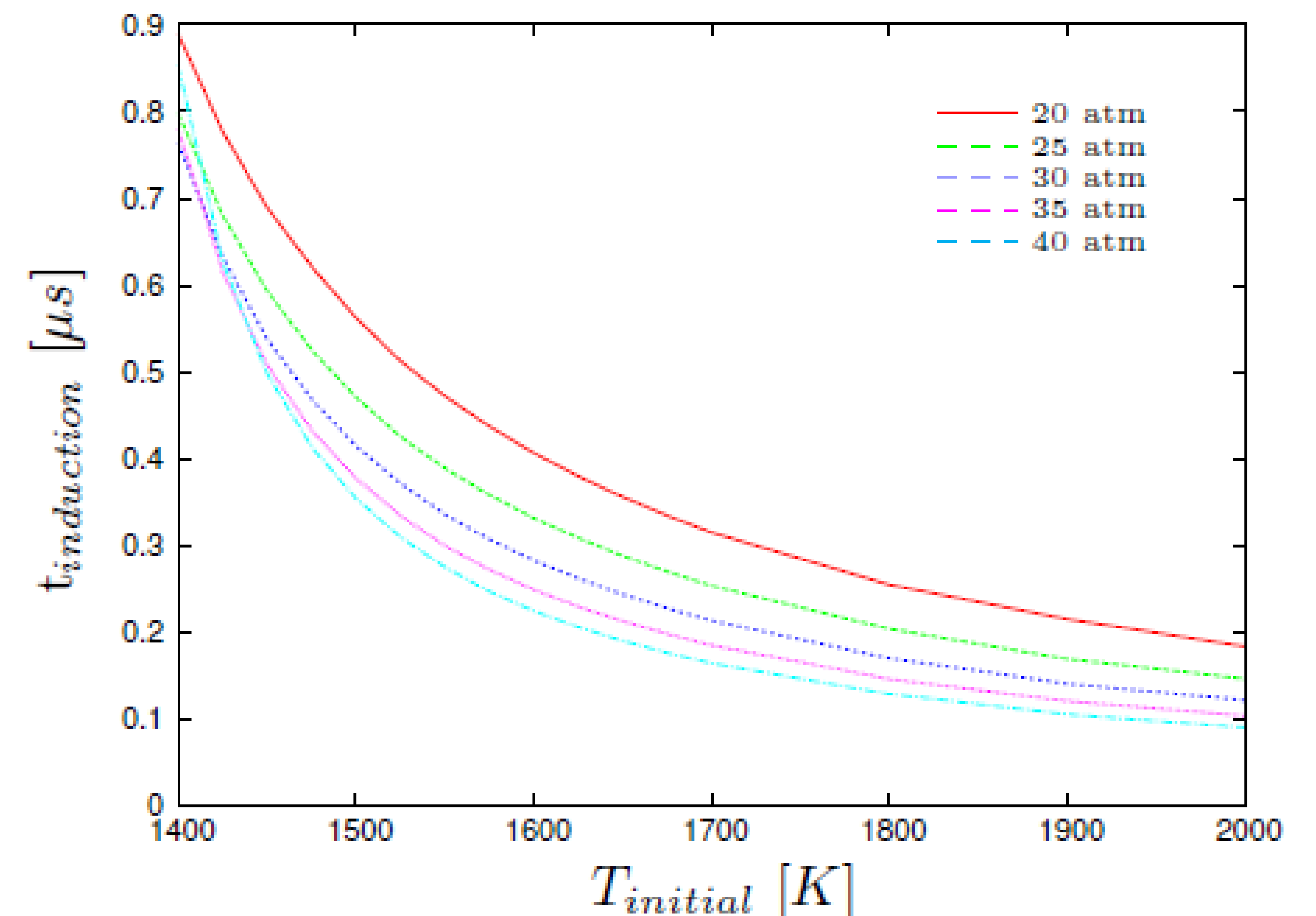
$$\frac{dn_k}{dt} = \sum_{j < k} \{ C_{kj}^{ex} n_e n_j - C_{jk}^{ed} n_e n_k - R_{jk} \} + \sum_h \sum_{j > k} \{ C_{kj}^{ed} n_e n_j - C_{jk}^{ex} n_e n_k + R_{kj} \}$$

$$\sum_{j < k} \{ C_{kj}^{hx} n_h n_j - C_{jk}^{hd} n_h n_k \} + \sum_h \sum_{j > k} \{ C_{kj}^{hd} n_h n_j - C_{jk}^{hx} n_h n_k \}$$

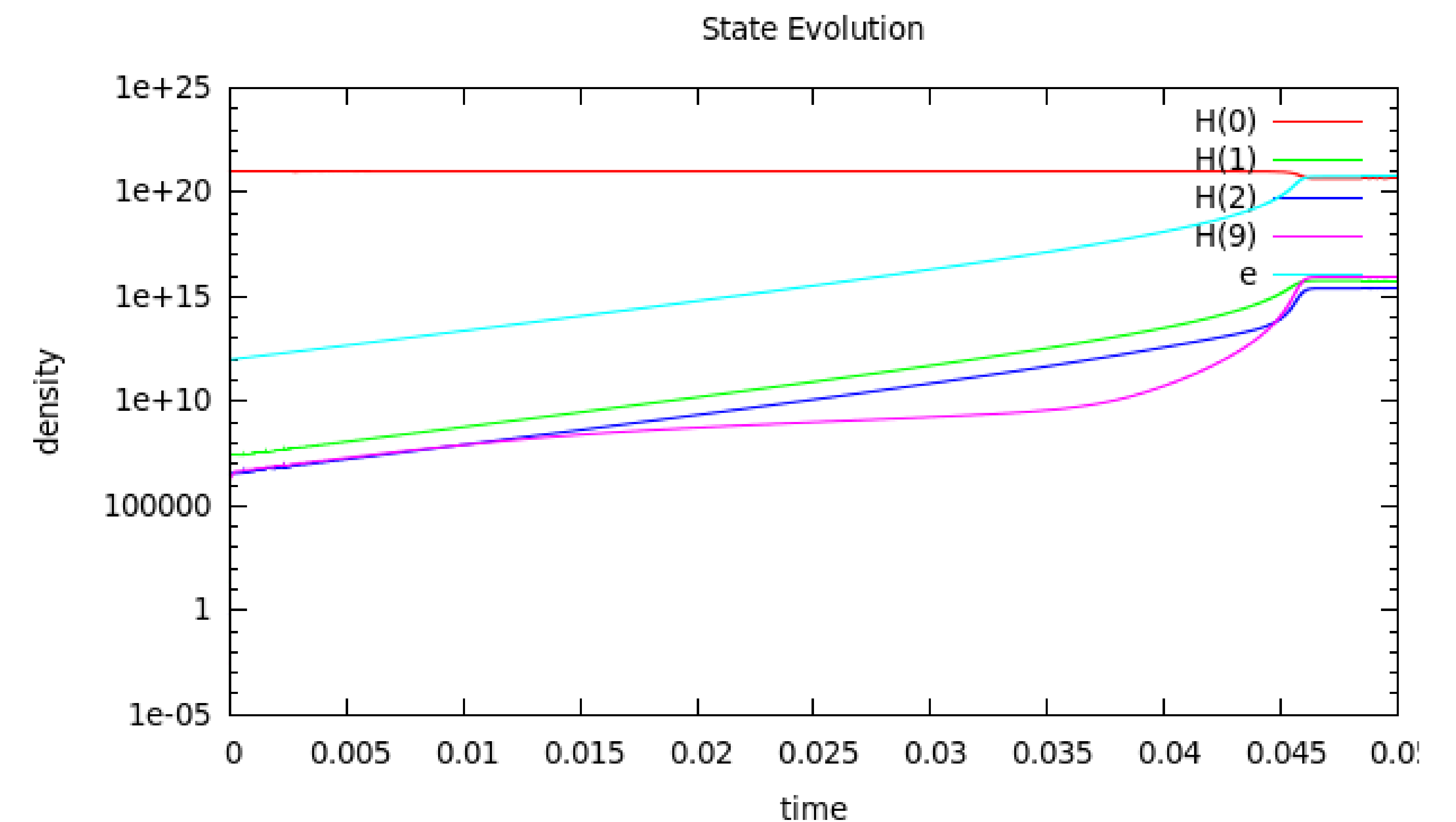
$$- C_k^{ei} n_e n_k + C_k^{er} n_e^2 n_i - \sum_h C_k^{hi} n_h n_k + \sum_h C_k^{hr} n_e n_h n_i + R_k n_e n_i$$

- Implicit kinetics solver

$$\frac{d\mathbf{Q}^n}{dt} = \dot{\mathbf{Q}}^{n+1} \rightarrow \left(I - \Delta t \frac{\partial \dot{\mathbf{Q}}}{\partial \mathbf{Q}} \right) \frac{d\mathbf{Q}^n}{dt} = \dot{\mathbf{Q}}^n$$



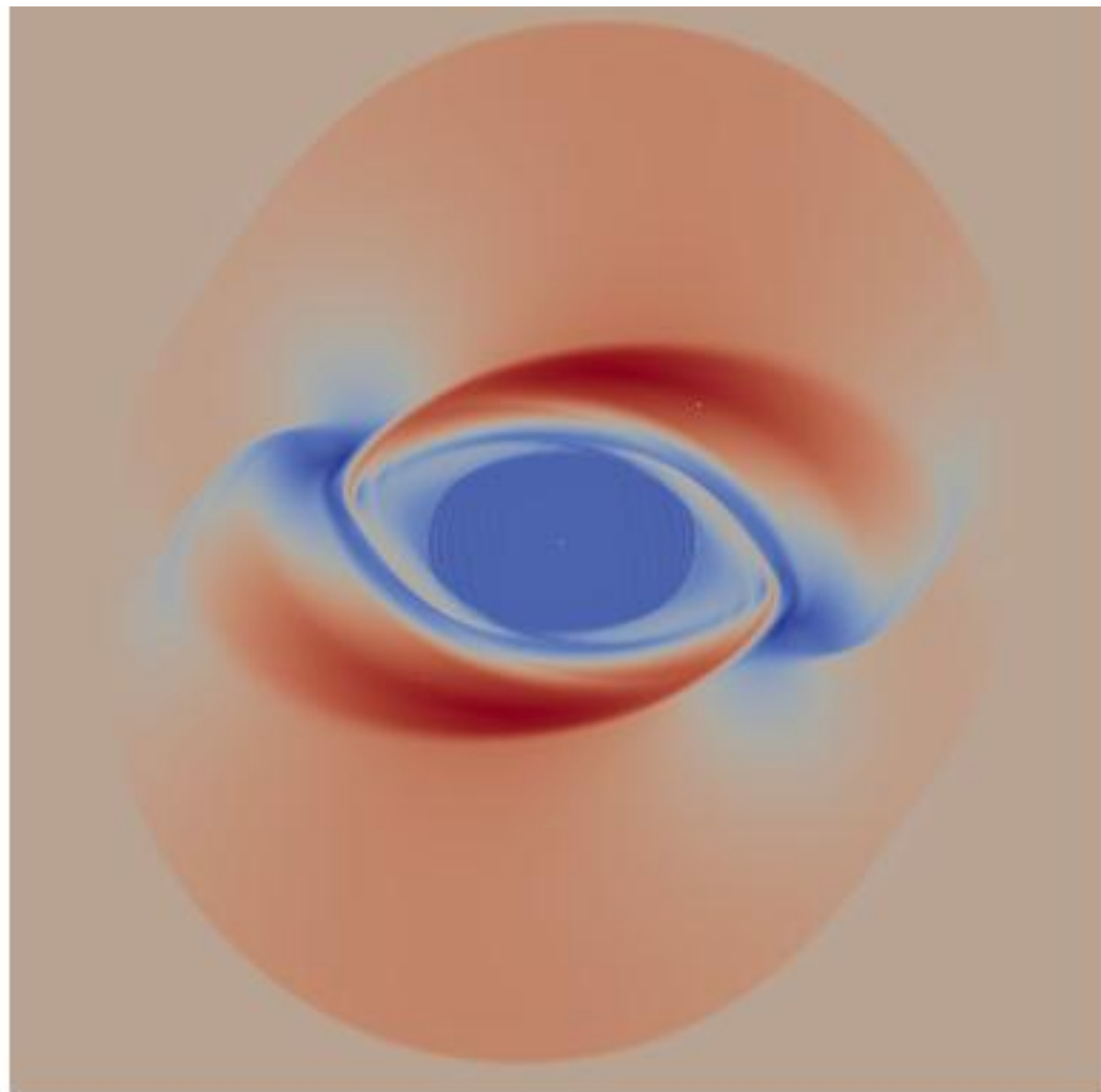
Induction delay time for Air mixture at various pressure and temperature



CR kinetics of electronic states of atomic hydrogen during isothermal heating process

Magnetohydrodynamic Simulations

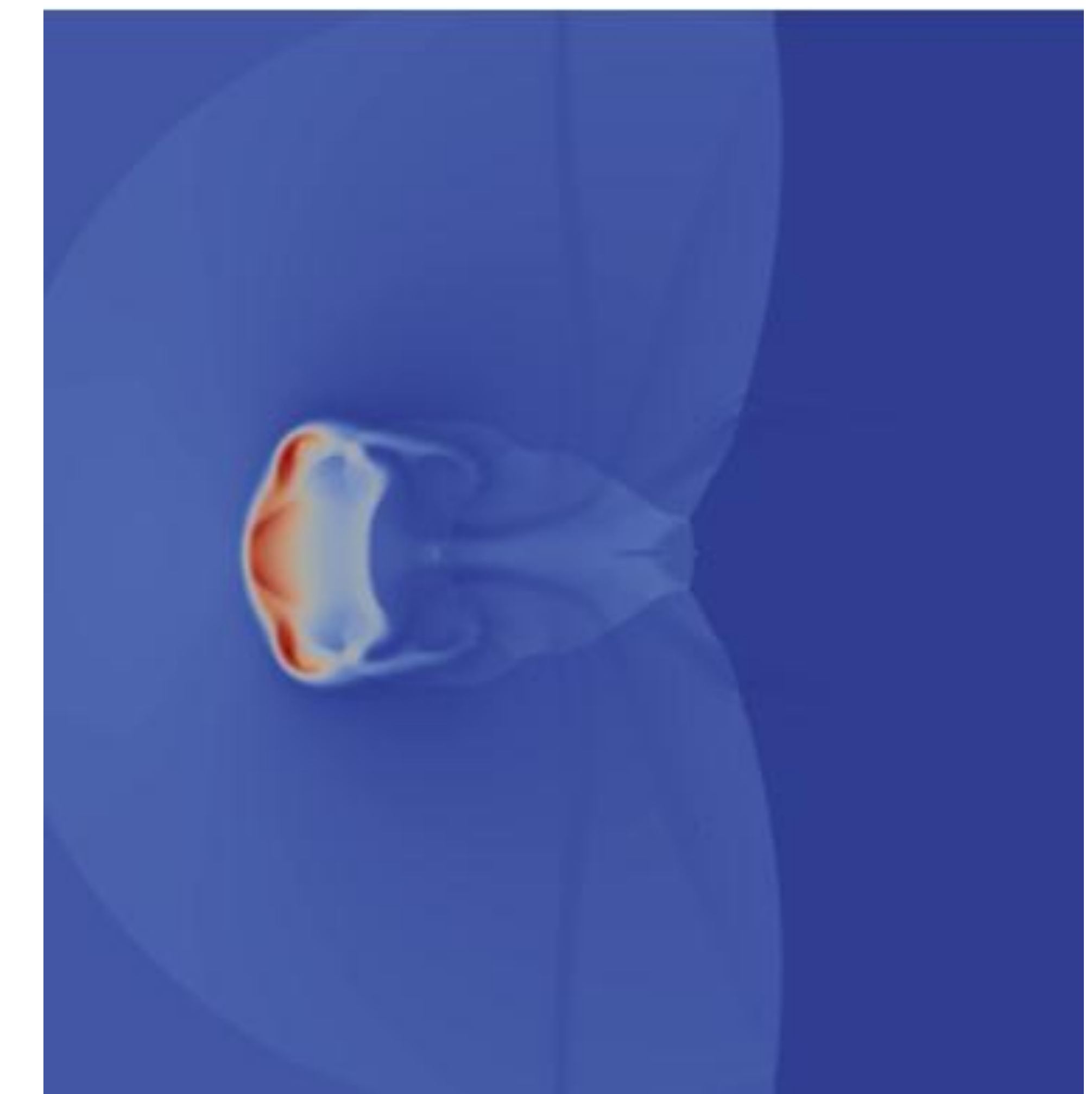
- Ideal MHD test cases



Rotor problem
(16,000 cells)



Orszag-Tang problem
(16,000 cells)



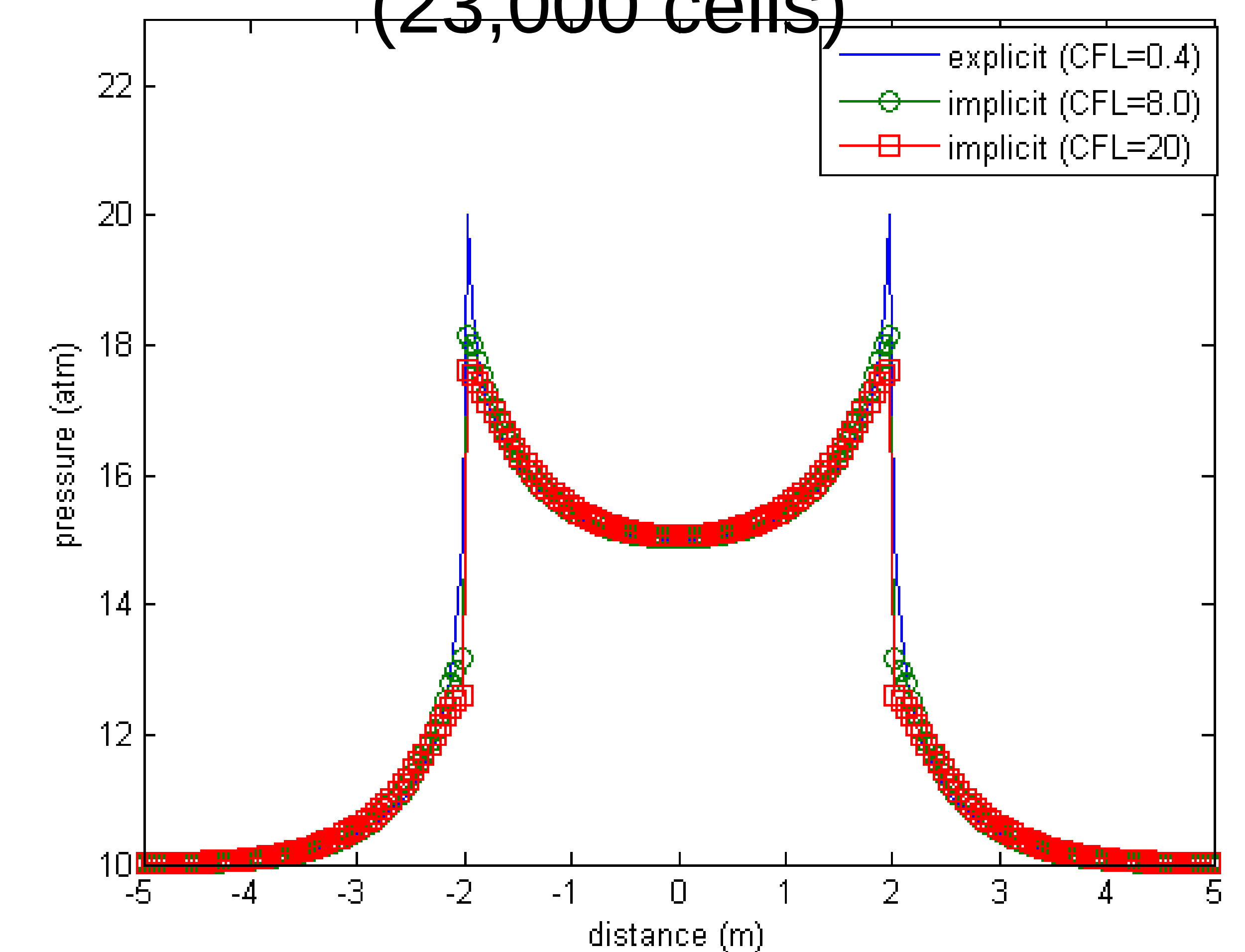
MHD cloud shock
(23,000 cells)

- Resistive MHD

$$\frac{\partial B^\alpha}{\partial t} + \nabla_\beta [u^\beta B^\alpha - u^\alpha B^\beta] = \nabla_\beta \left[\frac{1}{\sigma \mu_0} (\nabla^\beta B^\alpha - \nabla^\alpha B^\beta) \right]$$

$$\frac{\partial}{\partial t} [E_P + E_M] + \nabla_\beta [u^\beta (E_P + E_M) + u^\alpha (\bar{P}^{\alpha\beta} + T_M^{\alpha\beta})] = \nabla_\alpha \left[\frac{1}{\sigma \mu_0} \nabla_\beta T_M^{\alpha\beta} \right]$$

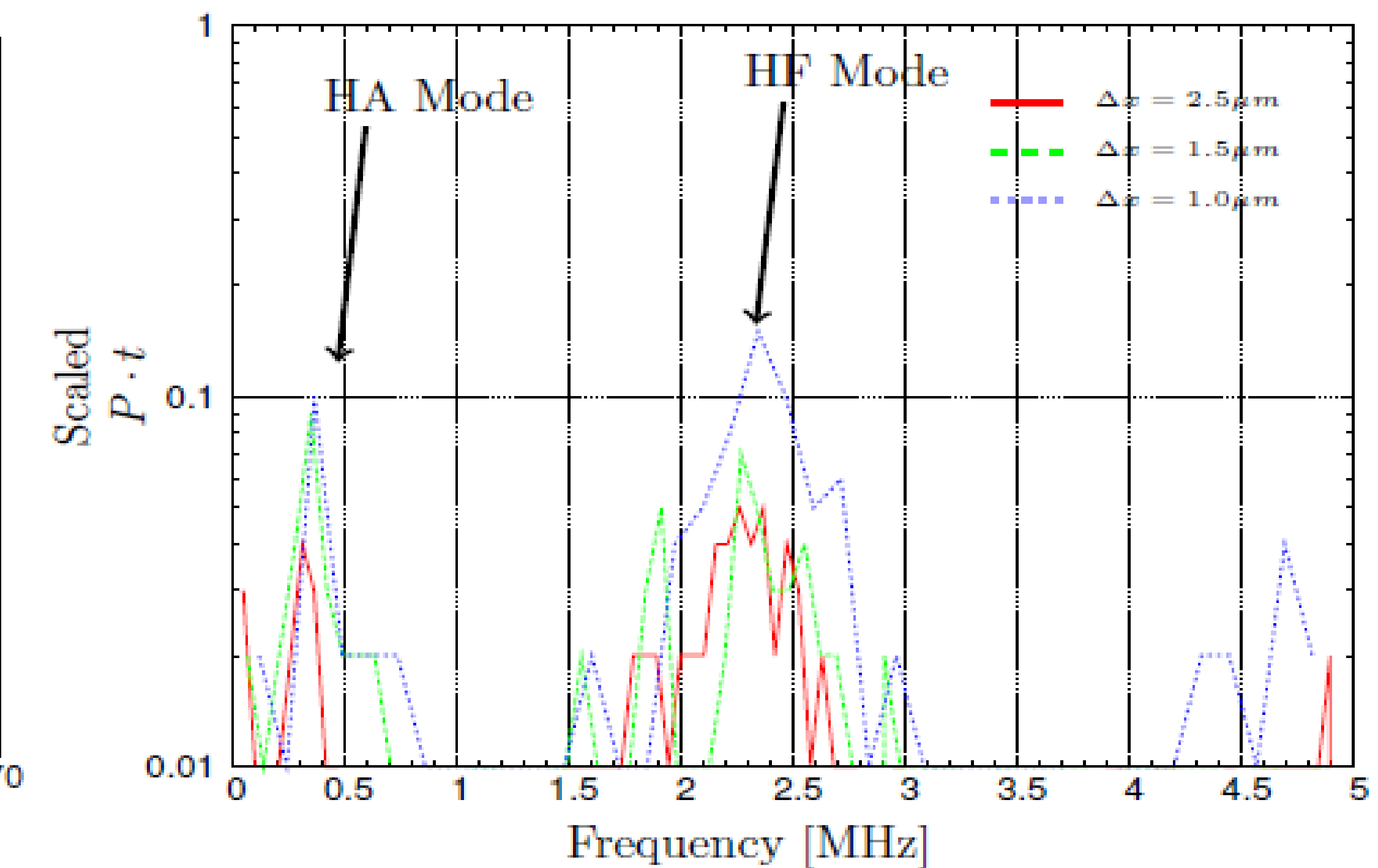
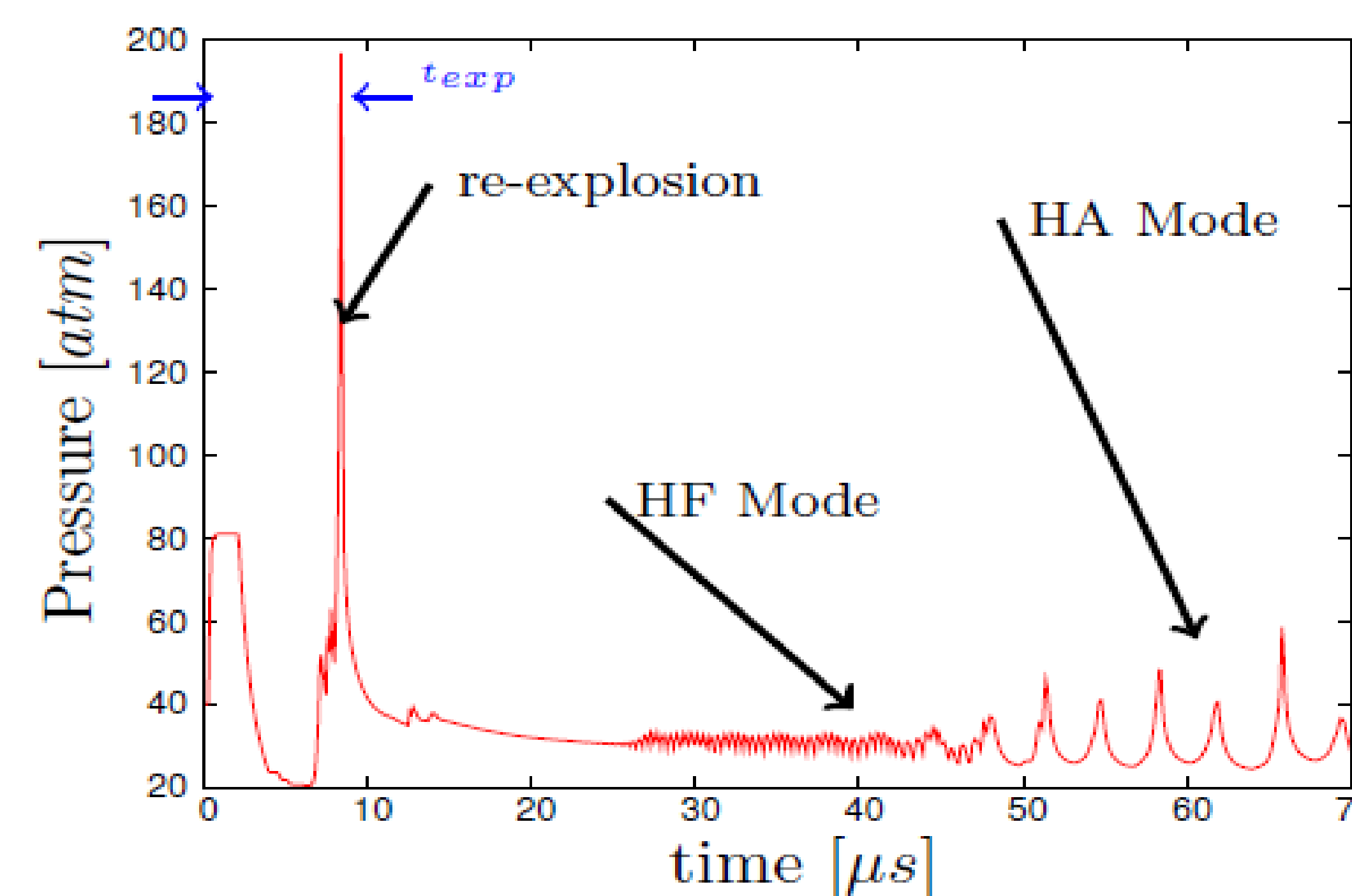
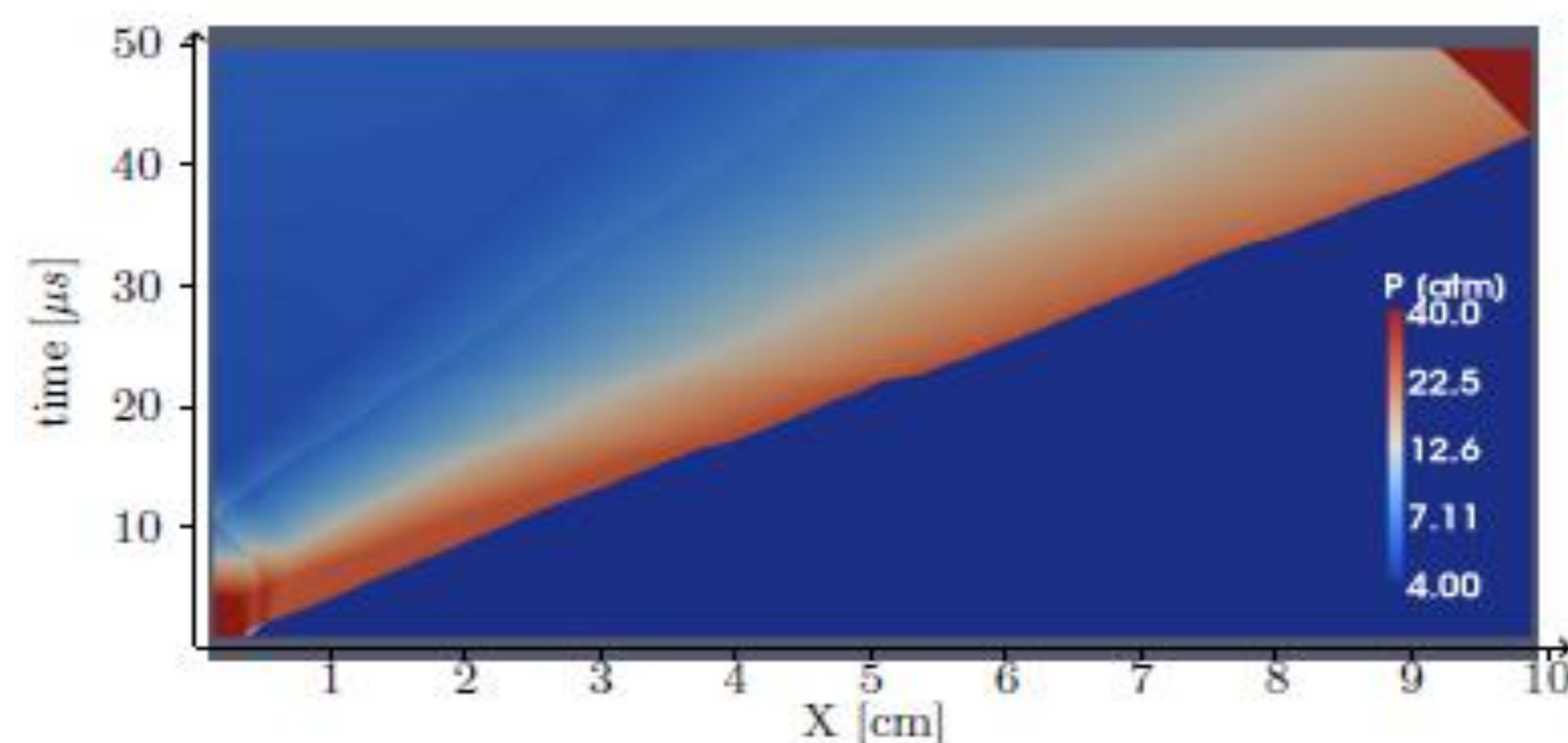
$$T_M^{\alpha\beta} = \frac{\vec{B}^2}{2\mu_0} \delta_{\alpha\beta} - \frac{B_\alpha B_\beta}{\mu_0}$$



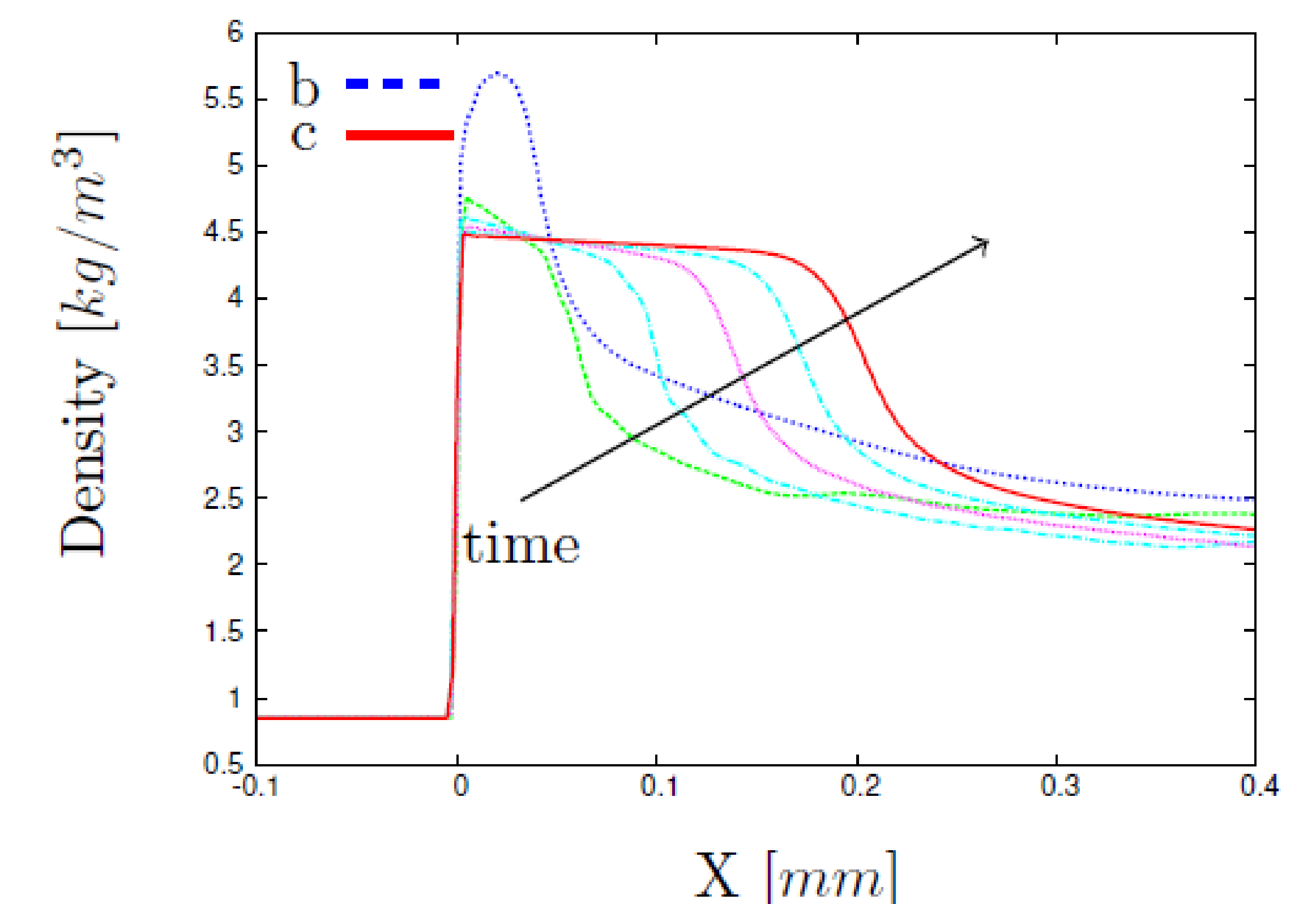
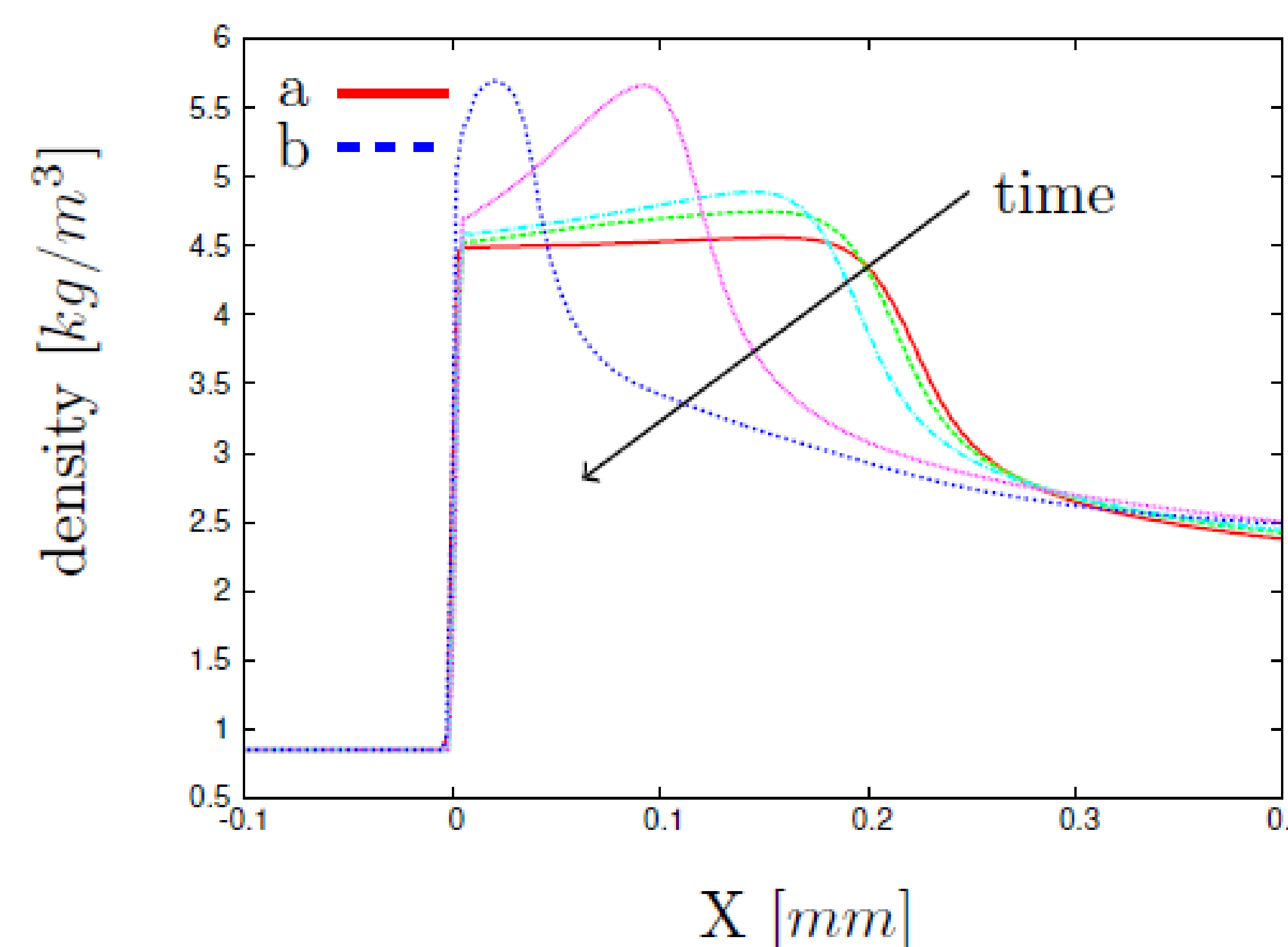
Comparison of heating rates (pressure rise) for explicit and implicit magnetic diffusion schemes

Flame-Shock Coupling: 1-D Dynamics of Instabilities

- Oscillatory patterns and distinct instability modes of a 1-D detonation wave at the CJ limit can be observed via high-order numerical simulation.
 - High frequency mode appears first and marks the transition from a stable CJ detonation
 - High amplitude (low frequency) mode appears later which directly couples the flame speed with the shock

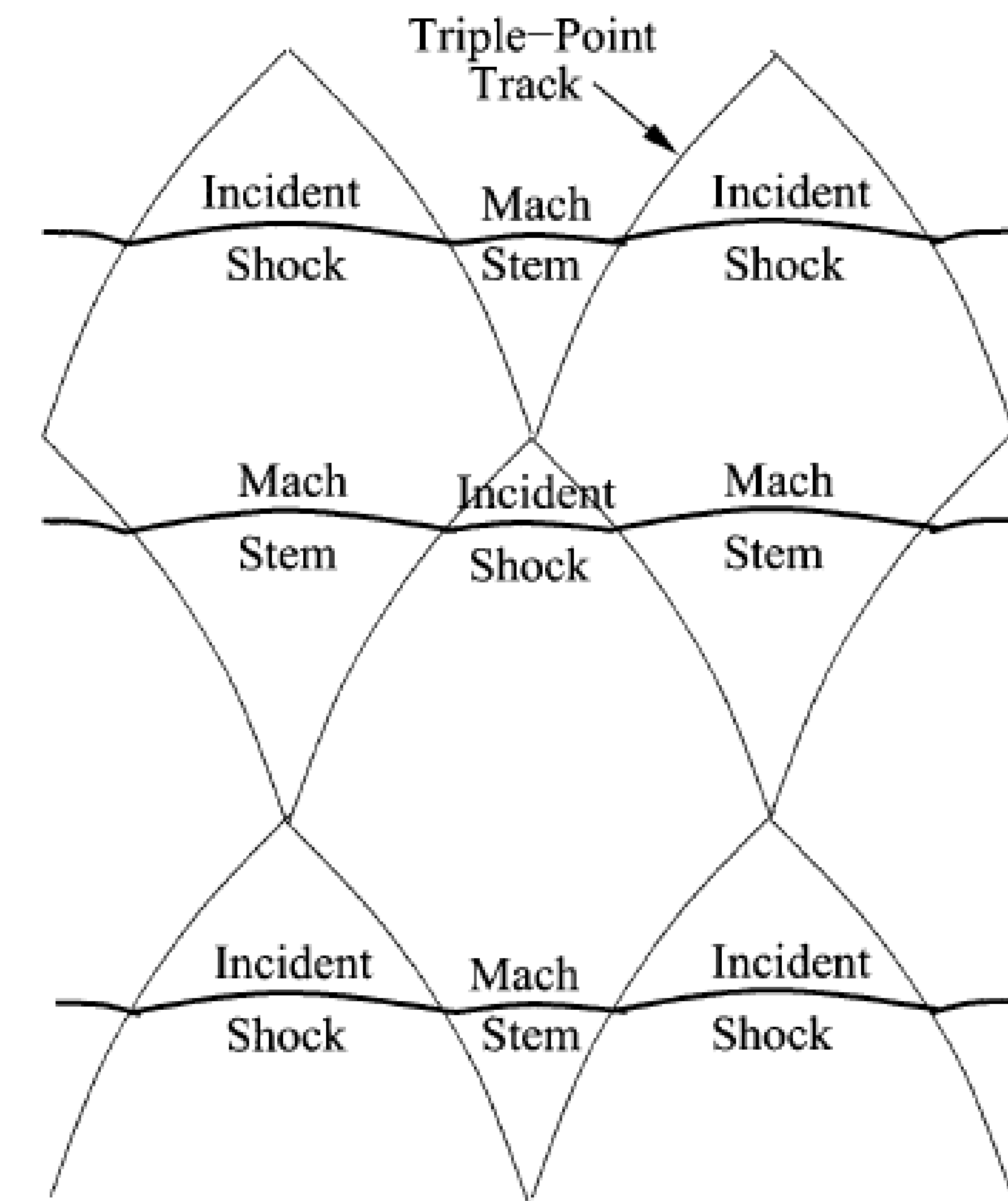


- The dynamics of a detonation wave can be explained by the strong coupling between fluid convection and kinetics.
 - Simple model: entropy and acoustic waves cycles in flame-shock coupling

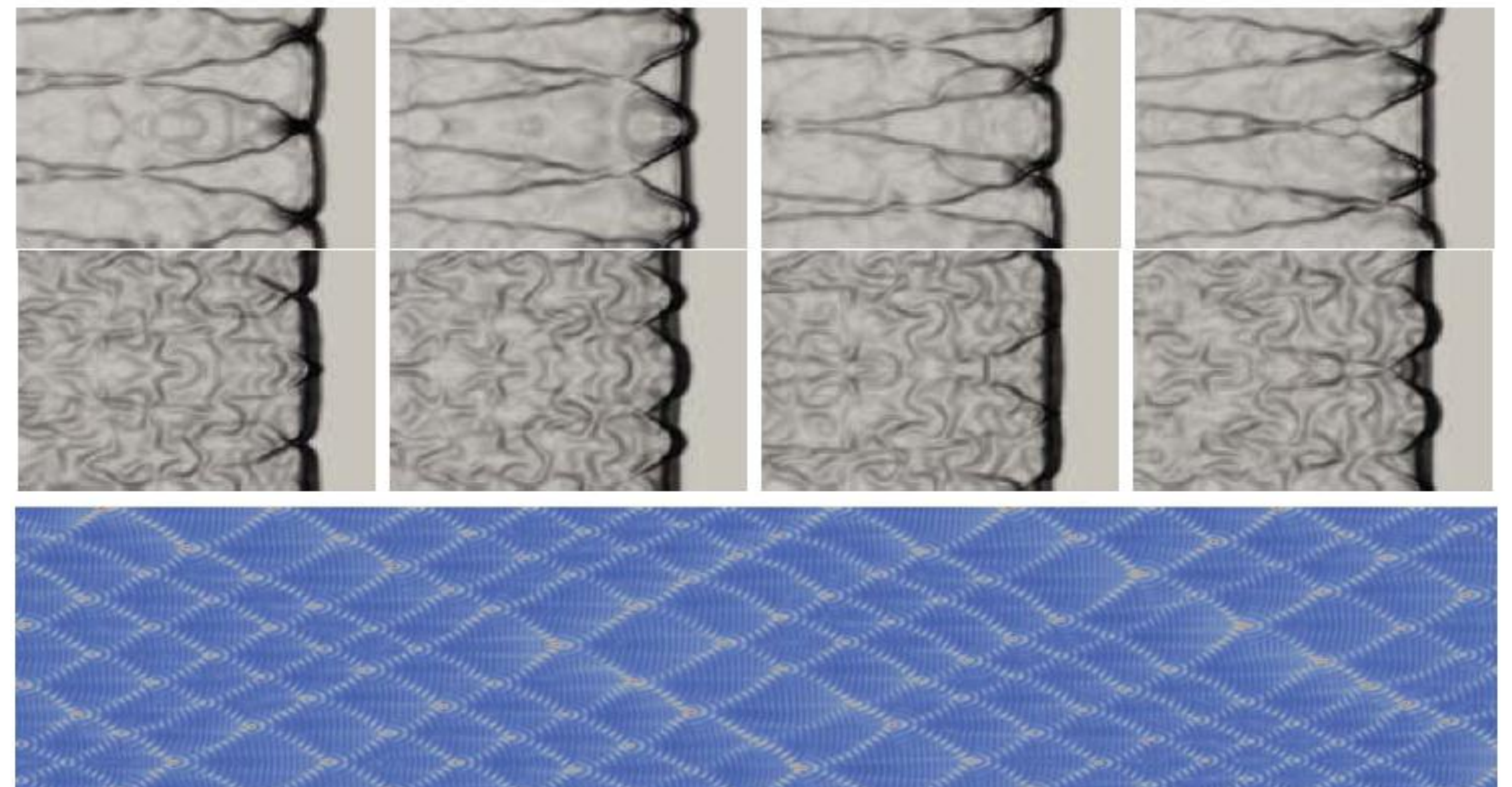


Flame-shock Coupling: Multi-dimensional Effects

- Influence of traverse waves
 - Unstable shock front due to interaction with the traverse waves.
 - The intersection of the lead shock and the traverse waves produces two triple points connected by a Mach stem that grows in width

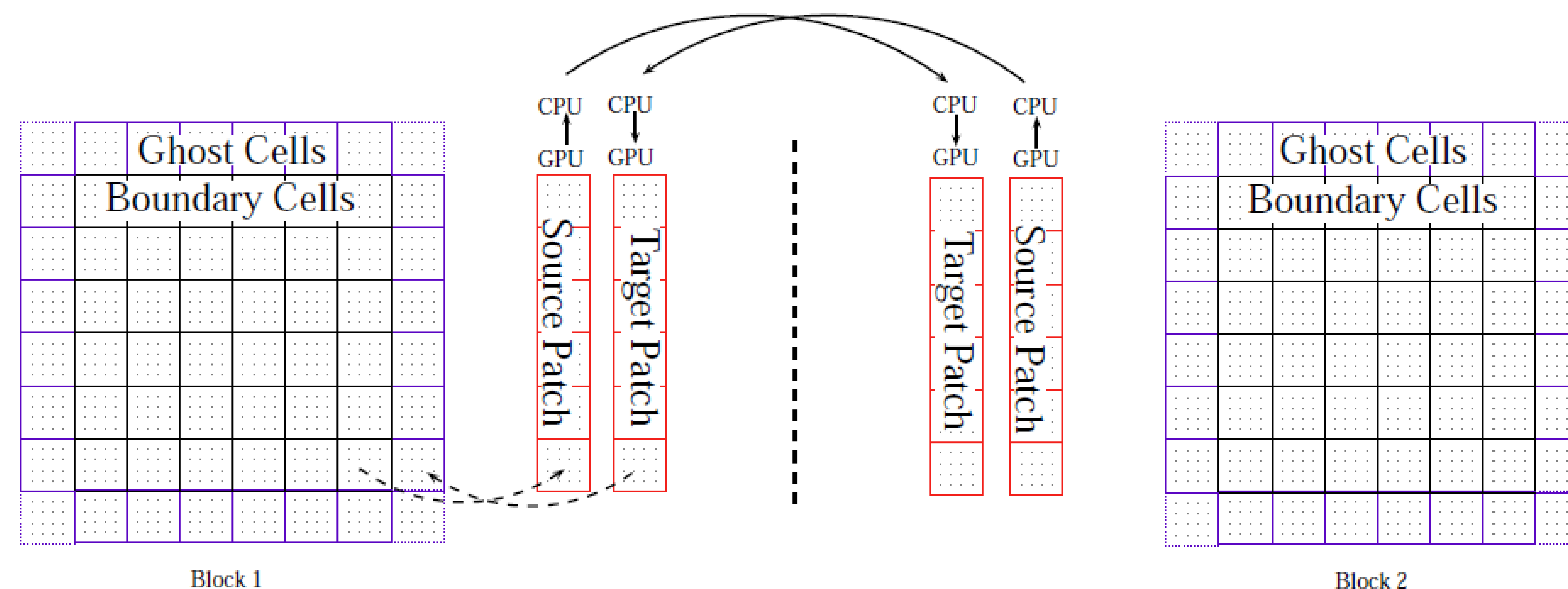


- Cellular pattern for 2D detonation simulation with complex kinetics
 - Characterize a network of triple points that are connected to smooth shock fronts



GPU parallelization

- Approaches
 - Cell-based (1 cell per thread) parallelization: EOS, time marching, chemistry, etc.
 - Face-based (1 face per thread) parallelization: Reconstruction, flux, etc.
- Optimization strategies
 - Coalesce memory access for optimal DRAM memory bandwidth
 - Utilize on-chip shared memory whenever possible
 - Reduce memory transfers between cpu and gpu
 - Adapt instruction level parallelism (ILP) within GPU kernels by reducing block occupancy and utilizing more registers
- Message passing interface (MPI) for multiGPU computation
 - Domain decomposition
 - Boundary exchange



GPU vs. CPU

Comparison between NVIDIA Tesla M2070 and Intel Xeon X5650 (single core comparison)

- Ideal Gas simulation (no chemical reaction)
 - 5th order accurate solutions (MP5 and ADERWENO)
 - Speedup factor up to 60
- Reacting flow simulation (detonation)
 - Comparison of two different mechanism: H₂-Air and CH₄-Air detonation
 - Speedup factor up to 40

