COMPUTER SIMULATIONS OF TWO DIMENSIONAL PLASMA EXPANSION DUE TO GRAPHITE TARGET ABLATION BY A NANOSECOND LASER PULSE

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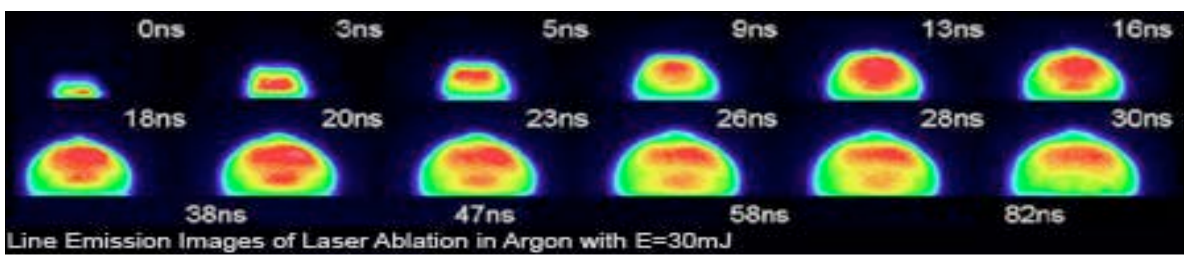
Laser Ablation

Process of removing material from a solid surface by striking it with a short laser pulse.

Ablated material converts to a plasma at high laser flux.

The plasma expands according to fluid dynamics equations.

Physiochemical experiments are difficult to implement.



Line Emission Images of Laser Ablation in Argon with E=30mJ

Applications

- Growing thin films
  - Plasma grows and covers the substrate.
  - Shock waves are detrimental to the film quality.
- Removal of material from a substrate
- Laser drilling
  - Dentistry
  - Surgery
  - Machinery

Numerical Goals

- Increase efficiency and resolution
- Multi-dimensional problems
- Increase accuracy of shock locations
- Parameter analysis
- Implementation of physically relevant initial conditions

Quasi-Gas Dynamics Model
Elizarova 2007

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{j}_m) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{j}_m) + \nabla p = \nabla \cdot \Pi$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{j}_m H) + \nabla \cdot \mathbf{q} = \nabla \cdot (\Pi \mathbf{u})$$

Quasi-Gas Dynamics Model
Mass Flux Density

$$\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w})$$

$$\mathbf{w} = \frac{\tau}{\rho}\left(\vec{\nabla}\cdot(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p - \rho\mathbf{F}\right)$$

In spatial-time averaging, the instantaneous values of momentum and density may change.
Therefore, we must express the mass flux density in a more general form by adding a term to the velocity that accounts for the gradient of the velocity vector.

Quasi-Gas Dynamics Model
Mass Flux Density

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$$\mathbf{w} = \frac{\tau}{\rho}\left(\vec{\nabla}\cdot(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p - \rho\mathbf{F}\right)$$

Quasi-Gas Dynamics Model
Mass Flux Density

$$\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w})$$

$$\mathbf{w} = \frac{\tau}{\rho}\left(\vec{\nabla}\cdot(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p - \rho\mathbf{F}\right)$$

$$\mathbf{j}_m = \rho\mathbf{u} - \tau\,\vec{\nabla}\cdot(\rho\mathbf{u}\otimes\mathbf{u}) - \tau RT\nabla\rho - \tau R\rho\nabla T + \tau\rho\mathbf{F}$$

Quasi-Gas Dynamics Model
Relaxation parameter

$$\mathbf{j}_m = \rho\mathbf{u} - \tau \vec{\nabla}\cdot(\rho\mathbf{u}\otimes\mathbf{u}) - \tau RT\nabla\rho - \tau R\rho\nabla T + \tau\rho\mathbf{F}$$

1. Convection
2. Gradient in velocity
3. Self-Diffusion
4. Thermo-Diffusion
5. Exterior forces

Quasi-Gas Dynamics Model
Relaxation parameter

$$\mathbf{j}_m = \rho\mathbf{u} - \tau\,\vec{\nabla}\cdot(\rho\mathbf{u}\otimes\mathbf{u}) - \tau RT\nabla\rho - \tau R\rho\nabla T + \tau\rho\mathbf{F}$$

Self-Diffusion Coefficient for polytropic gas: $D = \dfrac{\mu}{\rho \mathrm{Sc}}$

$$\tau = \frac{\mu}{\rho \mathrm{Sc}}\frac{1}{RT} = \frac{\mu}{p\,\mathrm{Sc}}$$

Quasi-Gas Dynamics Model Relaxation parameter

* When performing computer simulations *

- The Relaxation Parameter must no longer be related to the molecular properties of the gas.
- It may be determined by the step size, convergence conditions, and accuracy concerns of the numerical problem.

Quasi-Gas Dynamics – 1D

Elizarova 2007; Kuzyakov, Trofimov, Shirokov 2008

$$\frac{\partial \rho}{\partial t} + \frac{\partial j_m}{\partial x} = 0,$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (j_m u)}{\partial x} + \frac{\partial p}{\partial x} = \frac{\partial \Pi}{\partial x},$$

$$\frac{\partial E}{\partial t} + \frac{\partial (j_m H)}{\partial x} + \frac{\partial q}{\partial x} = \frac{\partial \Pi u}{\partial x},$$

$$j_m = \rho(u - w), \quad w = \frac{\tau}{\rho} \frac{\partial}{\partial x}(\rho u^2 + p)$$

Components

Equation of State

$$p = (\gamma - 1)\left[E - \frac{\rho u^2}{2} \right]$$

Ideal Gas Law

$$T = \frac{p}{\rho R}$$

Viscous Stress Tensor

$$\Pi = \Pi^{NS} + \tau\left[u\left(\rho u u_x + p_x \right) + \left(u p_x + \gamma p u_x \right) \right]$$

$$\Pi^{NS} = \left(\frac{4}{3}\eta + \eta\left(\frac{5}{3} - \gamma \right) B \right) \frac{\partial u}{\partial x}$$

Heat Flux

$$q = q^{NS} - \tau \rho u \left[\frac{u}{\gamma - 1} \frac{\partial}{\partial x}\left(\frac{p}{\rho} \right) + p u \frac{\partial}{\partial x}\left(\frac{1}{\rho} \right) \right]$$

$$q^{NS} = -\kappa T_x$$

Quasi-Gas Dynamics 1D Vector Form

$$\mathbf{u}_t + \mathbf{H}(\mathbf{u})_x = \mathbf{P}(\mathbf{u})$$

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}, \quad \mathbf{H}(\mathbf{u}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E + p)u \end{pmatrix}, \quad \mathbf{P}(\mathbf{u}) = \begin{pmatrix} \tau(\rho u^2 + p)_x \\ (\Pi + \rho w u)_x \\ (\Pi u - q + w(E + p))_x \end{pmatrix}_x$$

Semi-discrete Form - 1D

$$\frac{d}{dt}\bar{\mathbf{u}}_j(t) = -\frac{\mathbf{H}_{j+\frac{1}{2}}(t) - \mathbf{H}_{j-\frac{1}{2}}(t)}{\Delta x} + \frac{\mathbf{P}_{j+\frac{1}{2}}(t) - \mathbf{P}_{j-\frac{1}{2}}(t)}{\Delta x}$$

1. Hyperbolic Numerical Flux

2. Parabolic Numerical Flux

3. Temporal integration

Semi-discrete Form - 1D

$$\frac{d}{dt}\bar{\mathbf{u}}_j(t) = -\frac{\mathbf{H}_{j+\frac{1}{2}}(t) - \mathbf{H}_{j-\frac{1}{2}}(t)}{\Delta x} + \frac{\mathbf{P}_{j+\frac{1}{2}}(t) - \mathbf{P}_{j-\frac{1}{2}}(t)}{\Delta x}$$

1. Hyperbolic Numerical Flux

Semidiscrete Central-Upwind Scheme (Kurganov, et al., 2001)

2. Parabolic Numerical Flux

Second-order Central Differences

3. Temporal integration

SSP Runge-Kutta (Higueras, 2009)

DUMKA variable time-step stiff ODE solver (Medovikov, 1998)

Single Gas Problem

Initial Conditions on $0 \le x \le L = 0.2\,\mathrm{m}, \quad 0 \le t \le t_f = 4\mu s$

$$p(x,0) = \begin{cases} 10^8\ \mathrm{Pa}, & \text{if } x \le 5\times10^{-6} \\ 3\ \mathrm{Pa}, & \text{if } x > 5\times10^{-6} \end{cases}, \qquad T(x,0) = \begin{cases} 3\times10^4\ \mathrm{K}, & \text{if } x \le 5\times10^{-6} \\ 300\ \mathrm{K}, & \text{if } x > 5\times10^{-6} \end{cases}$$

Boundary Conditions

$$u = 0, \quad \frac{\delta\rho}{\delta x} = 0, \quad \frac{\delta T}{\delta x} = 0$$

Single Gas Problem

Relaxation Parameter

$$\tau = \frac{\alpha \Delta x}{\mathrm{Sc} \cdot c}$$

Computational Parameters and Run Times (N=5000)

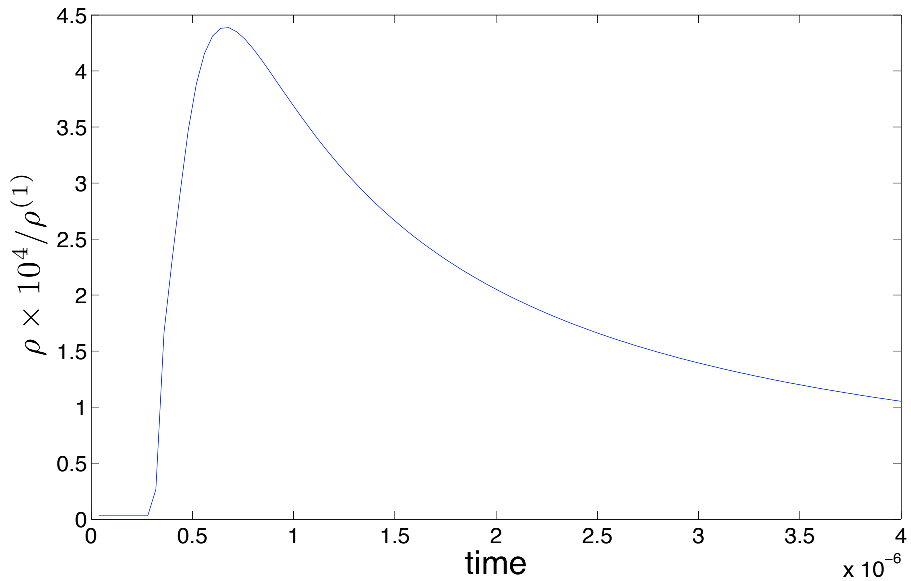
	θ	α	c_1	c_2	Run Time
1	1.3	0.6	0.45	0.5	34m 52.381s
2	1.55	0.6	0.45	0.5	34m 22.113s
3	1.55	0.6	0.45	1.0	17m 16.509s
4	1.55	0.6	0.45	1.65	10m 36.695s
5	1.55	0.275	0.45	1.65	10m 44.895s

Results – QGD

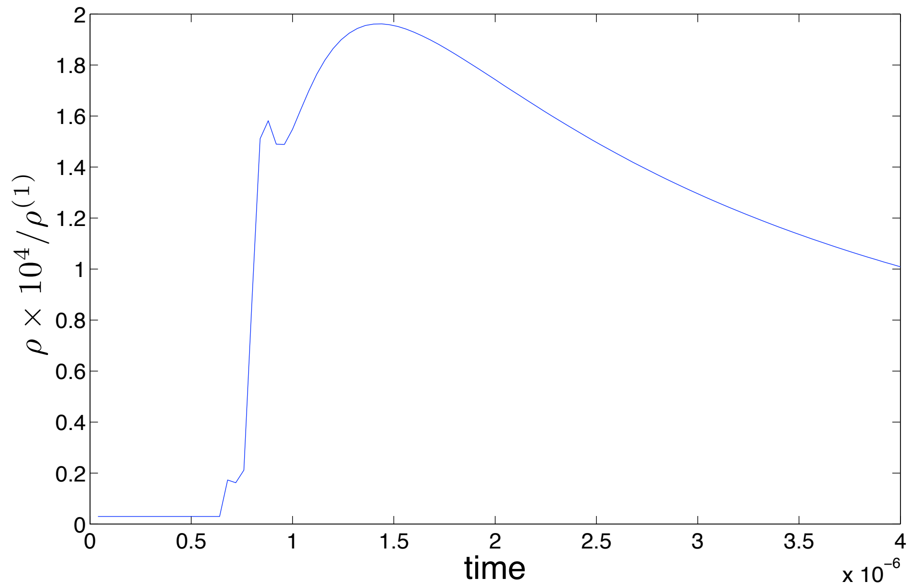
$$N = 5000, \quad \Delta x = 4\times10^{-6}, \quad t_f = 4\times10^{-6}\ \mathrm{s}$$

Normalized Density vs. Time

$x = 5\ \mathrm{mm}$



$x = 11\ \mathrm{mm}$

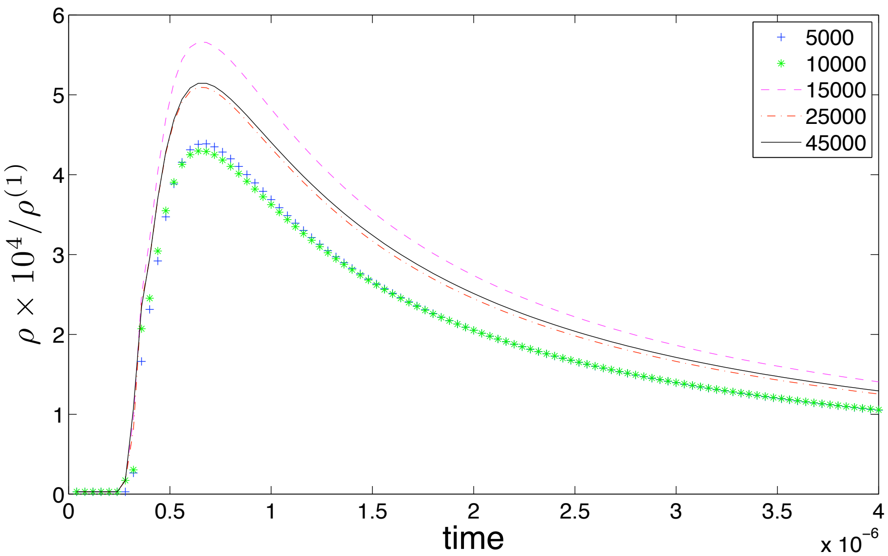


Results – QGD 1D Convergence

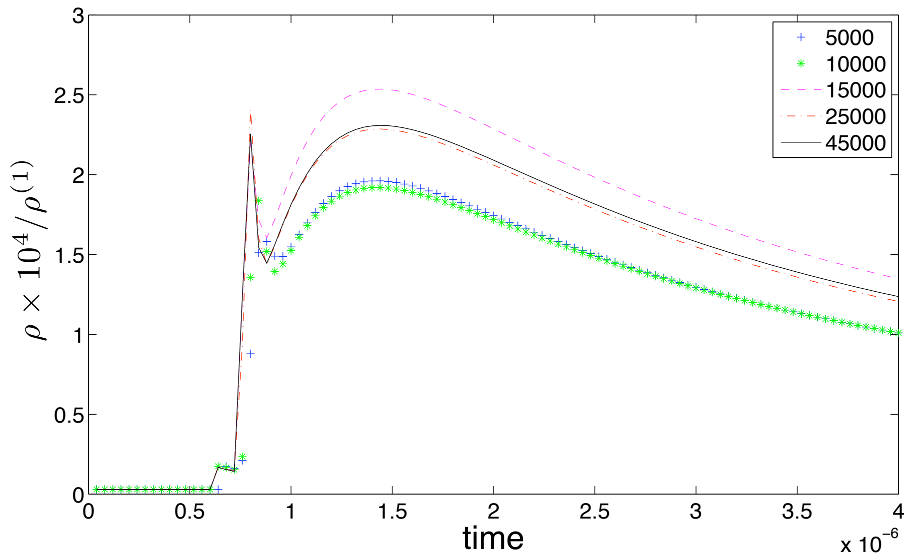
$\Delta x = 4 \times 10^{-6}, \quad t_f = 4 \times 10^{-6}$ s

Normalized Density vs. Time

$x = 5$ mm



$x = 11$ mm

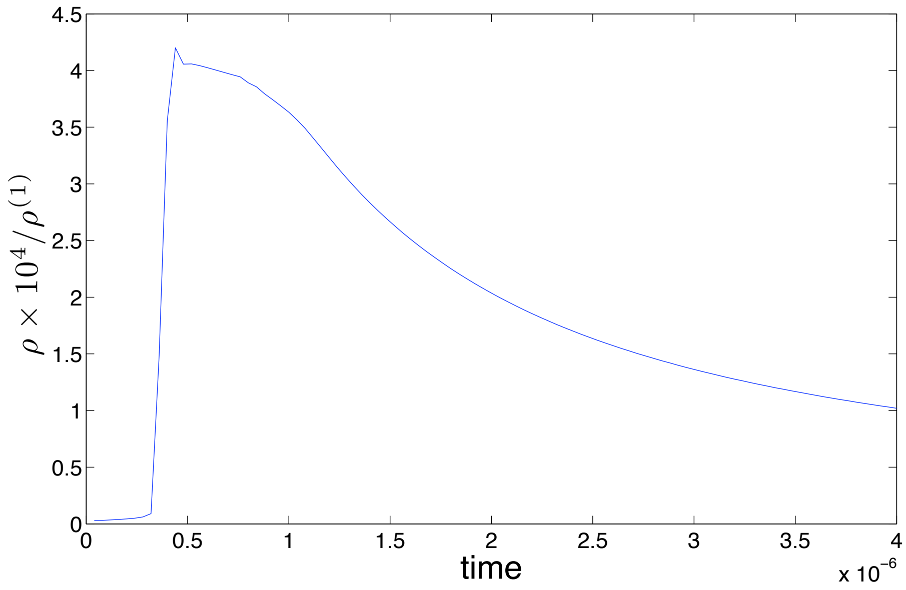


Results – Navier-Stokes

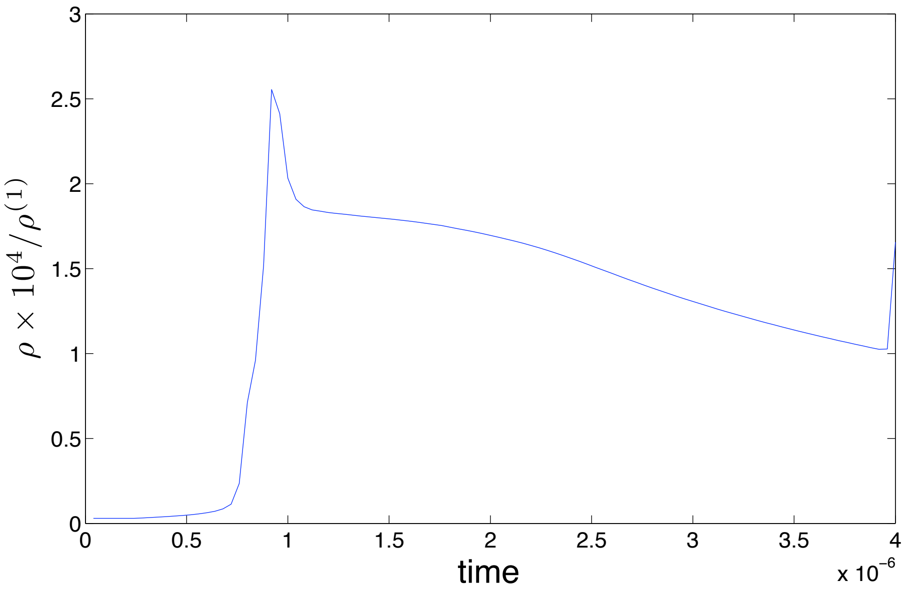
$$N = 5000, \quad \Delta x = 4 \times 10^{-6}, \quad t_f = 4 \times 10^{-6}\ \text{s}$$

Normalized Density vs. Time

$x = 5\ \text{mm}$

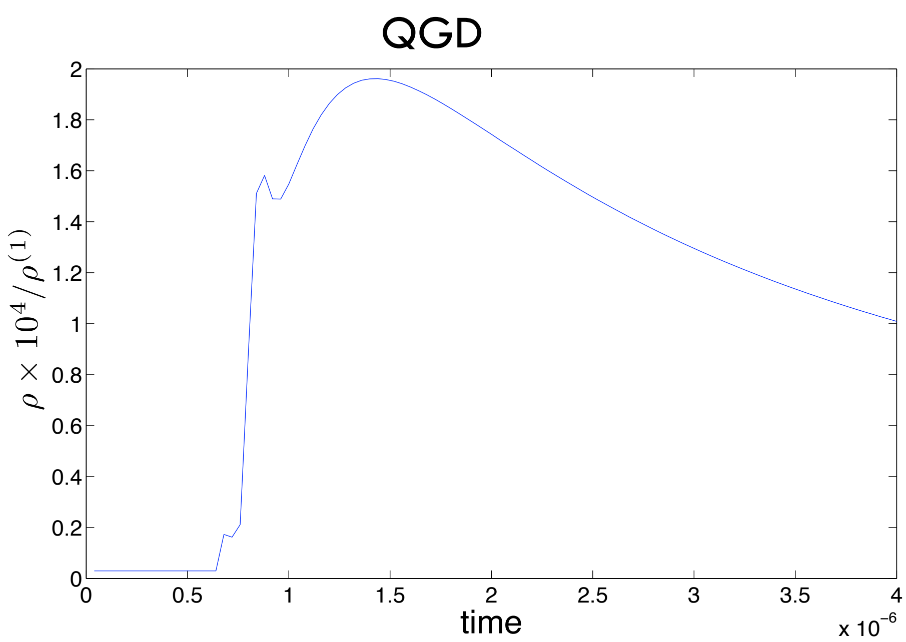


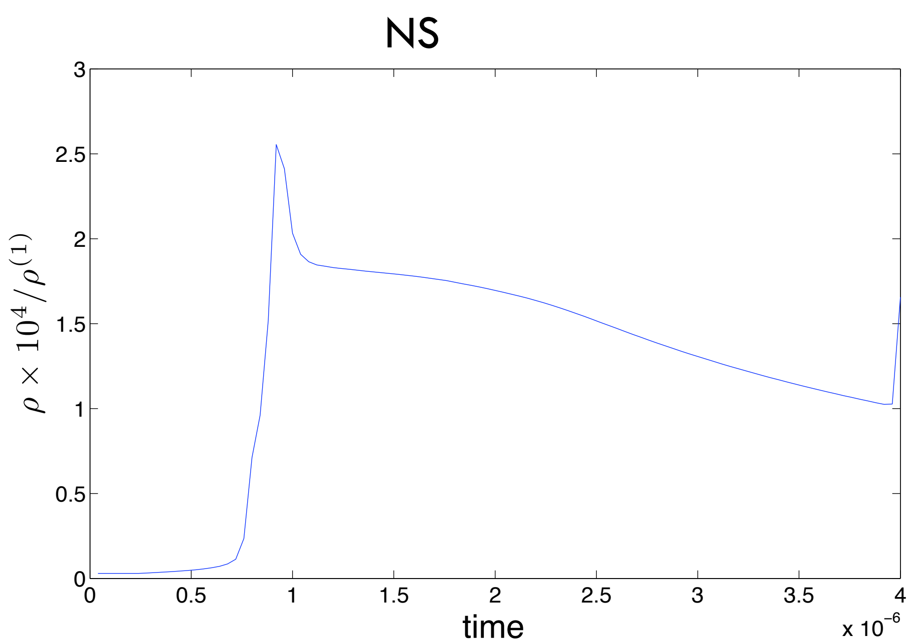
$x = 11\ \text{mm}$



Tau Analysis

We should get the NS equations as $\tau \to 0$



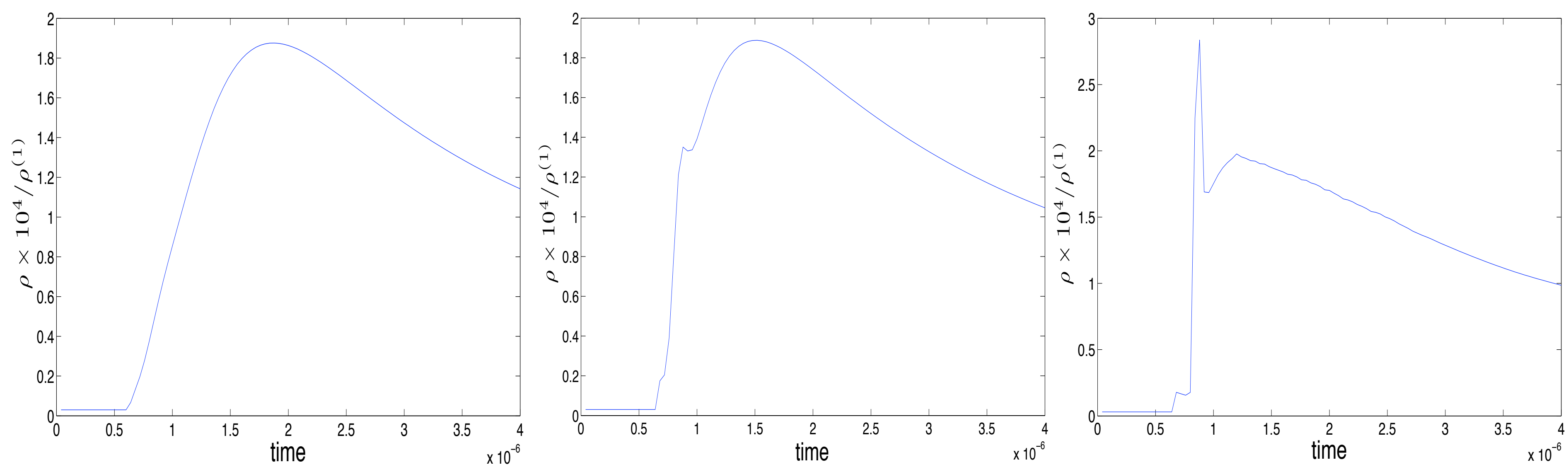


$$x = 11\,\mathrm{mm}$$

Constant Tau Results

We should get the NS equations as $\tau \to 0$

$\tau = 10^{-8}$ $\tau = 10^{-9}$ $\tau = 10^{-10}$



$$x = 11\,mm$$

Run Time Comparison

… and we get significant savings over Navier-Stokes:

- QGD simulations – 10-30 minutes.
- Constant tau simulations – 30 – 80 minutes.
- Navier Stokes simulation – 38 HOURS.

Quasi-Gas Dynamics – 1D Single Gas Further Experiments

- Varying the size of the strike zone affects the speed of the expansion and the size of the shock front.
- When the initial pressure in the strike zone is raised to experimentally significant magnitude, we were able to resolve solutions with a more realistic initial pressure in the expansion atmosphere – thus more realistically modeling the physical experiments.

$$p^{(1)} \sim \mathcal{O}(10^{10}), \quad p^{(2)} \sim \mathcal{O}(1)$$

Quasi-Gas Dynamics – 1D Binary Gas

Trofimov, Shirokov 2009

- More realistically, we model the expansion of the carbon laser plasma into a nitrogen atmosphere.
- The QGD equations are used to model the expansion for each gas.
- The systems are coupled together via momentum and energy exchange terms.
- Analysis allows one to determine the minimum pressure at which the buffer gas begins to adversely affect the the carbon expansion.

Momentum and Energy Exchange

The exchange terms are calculated as follows:

$$S_a^u = \nu_{ab}\rho_a(\bar{u}_a - u_a),$$

$$S_a^E = \nu_{ab}(\bar{E}_a - E_a),$$

$$S_b^u = -S_a^u,$$

$$S_b^E = -S_a^E.$$

The frequency of collisions between molecules of gases:

$$\nu_{ab} = \frac{p_a}{\eta_a^*}\Omega_a\sqrt{\frac{M_a + M_b}{2M_b}}\frac{\rho_b}{\rho_a}\frac{M_a}{M_b}$$

Quasi-Gas Dynamics – 1D Binary Gas

$$\frac{\partial \rho_a}{\partial t} + \frac{\partial j_a}{\partial x} = 0,$$

$$\frac{\partial (\rho_a u_a)}{\partial t} + \frac{\partial (j_a u_a)}{\partial x} + \frac{\partial p_a}{\partial x} = \frac{\partial \Pi_a}{\partial x} + S_a^u,$$

$$\frac{\partial E_a}{\partial t} + \frac{\partial (j_a H_a)}{\partial x} + \frac{\partial q_a}{\partial x} = \frac{\partial \Pi_a u_a}{\partial x} + S_a^E,$$

$$j_a = \rho_a (u_a - w_a), \quad w_a = \frac{\tau_a}{\rho_a} \frac{\partial}{\partial x} (\rho_a u_a^2 + p_a)$$

1D Binary Gas Problem

Initial Conditions on $0 \le x \le L = 0.2\,\text{m}, \quad 0 \le t \le t_f = 4\mu s$

$$(p_a(x,0), T_a(x,0), u_a(x,0)) = (p_a, T_a, 0), \quad 0 \le x \le 0.02\,\text{m}$$

$$(p_b(x,0), T_b(x,0), u_b(x,0)) = \begin{cases} (p_b^{(1)}, T_b^{(1)}, 0), & \text{if } x \le 5\times 10^{-6}\,\text{m}, \\ (p_b^{(2)}, T_b^{(2)}, 0), & \text{if } x > 5\times 10^{-6}\,\text{m}. \end{cases}$$

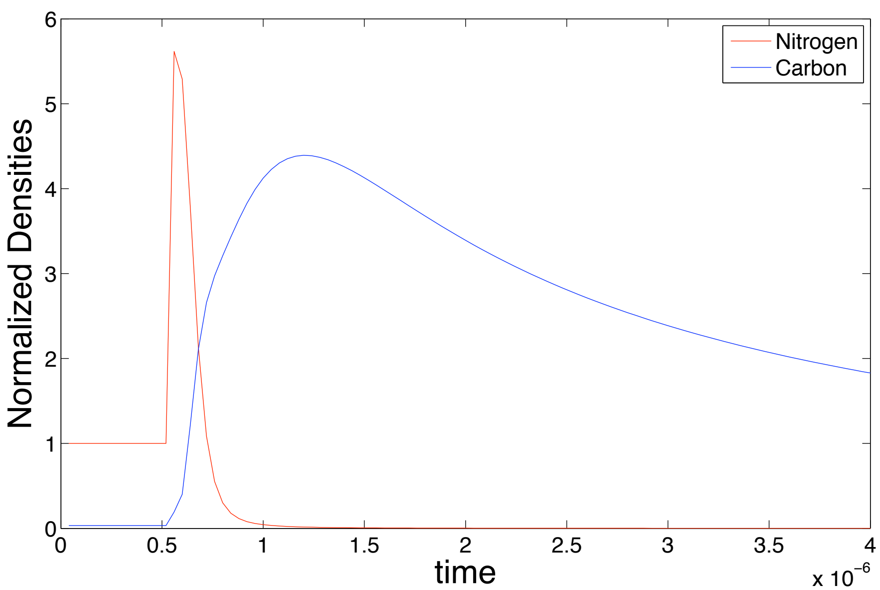
$$T_a = 300\,\text{K}, \quad p_b^{(2)} = 10^3\,\text{Pa}, \quad T_b^{(2)} = 300\,\text{K}$$

Boundary Conditions

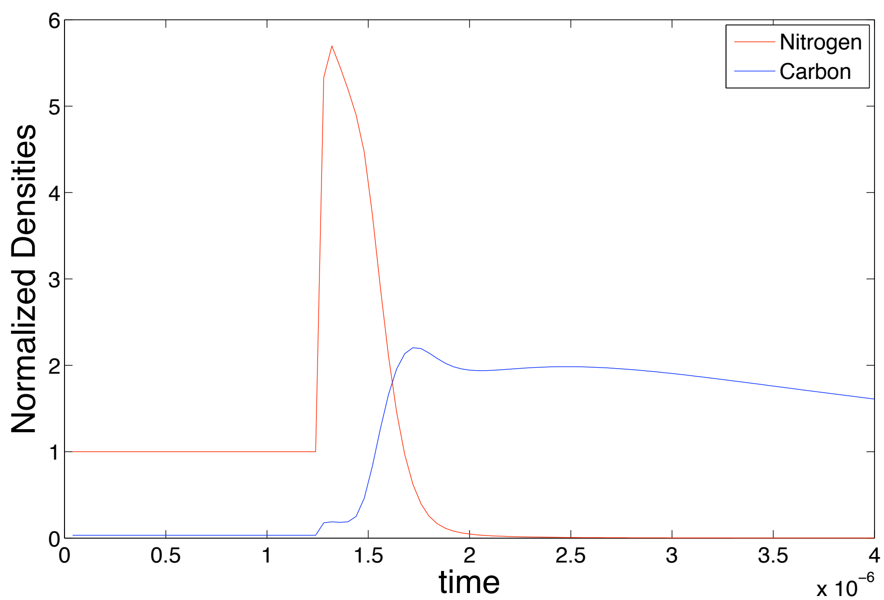
$$u = 0, \quad \frac{\delta\rho}{\delta x} = 0, \quad \frac{\delta T}{\delta x} = 0$$

1D Binary Gas – Results: Version 1

$x = 5\ \mathrm{mm}$



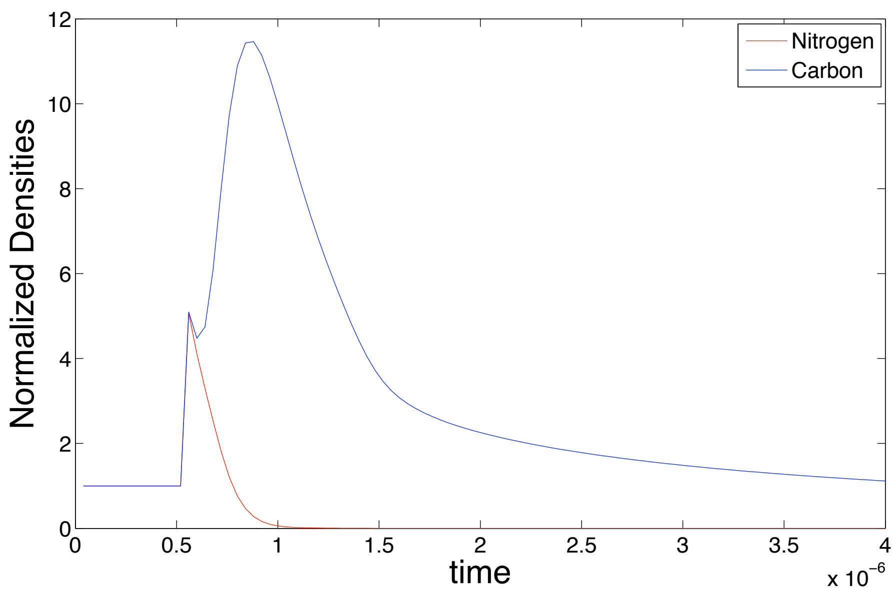
$x = 11\ \mathrm{mm}$



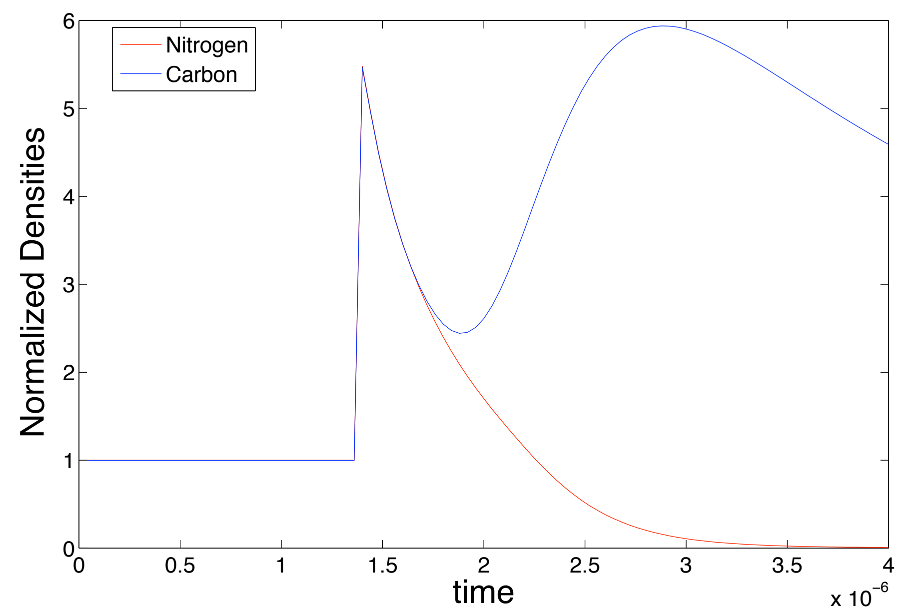
$$p_a = 10^3\ \mathrm{Pa}, \quad p_b^{(1)} = 10^{10}\ \mathrm{Pa}, \quad T_b^{(1)} = 10^4\ \mathrm{K}$$

1D Binary Gas – Results: Version 3

$x = 5$ mm



$x = 11$ mm



$$p_a = 10^3 \text{ Pa}, \quad p_b^{(1)} = 10^9 \text{ Pa}, \quad T_b^{(1)} = 3 \times 10^4 \text{ K}$$

2D Quasi-Gas Dynamics

- The two-dimensional QGD model is computationally exhaustive.
- The semi-discrete scheme is able to resolve the (more lenient) 2D initial conditions with a 400x400 grid.
- The 2D QGD simulation of the laser ablation problem had not been executed previously.

2D Quasi-Gas Dynamics

$$\frac{\partial \rho}{\partial t} + \frac{\partial j^{(x)}}{\partial x} + \frac{\partial j^{(y)}}{\partial y} = 0$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(j^{(x)}u)}{\partial x} + \frac{\partial(j^{(y)}u)}{\partial y} + \frac{\partial p}{\partial x} = \frac{\partial \Pi^{(xx)}}{\partial x} + \frac{\partial \Pi^{(yx)}}{\partial y}$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(j^{(x)}v)}{\partial x} + \frac{\partial(j^{(y)}v)}{\partial y} + \frac{\partial p}{\partial y} = \frac{\partial \Pi^{(xy)}}{\partial x} + \frac{\partial \Pi^{(yy)}}{\partial y}$$

$$\frac{\partial E}{\partial t} + \frac{\partial(j^{(x)}H)}{\partial x} + \frac{\partial(j^{(y)}H)}{\partial y} + \frac{\partial q^{(x)}}{\partial x} + \frac{\partial q^{(y)}}{\partial y} = \frac{\partial}{\partial x}\left(\Pi^{(xx)}u + \Pi^{(xy)}v\right) + \frac{\partial}{\partial y}\left(\Pi^{(yx)}u + \Pi^{(yy)}v\right)$$

$$j^{(x)} = \rho(u - w^{(x)}), \quad w^{(x)} = \frac{\tau}{\rho}\left[\frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} + \frac{\partial p}{\partial x}\right]$$

$$j^{(y)} = \rho(v - w^{(y)}), \quad w^{(y)} = \frac{\tau}{\rho}\left[\frac{\partial(\rho u v)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial p}{\partial y}\right]$$

Viscosity Tensors and Heat Flux

Viscosity

$$\Pi^{(xx)} = \mu\left(2\frac{\partial u}{\partial x} - \left[\frac{2}{3} - \frac{\zeta}{\mu}\right]\operatorname{div}\vec{u}\right) + \tau\gamma p \operatorname{div}\vec{u} + \tau\rho u\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) + \tau\left(2u\frac{\partial p}{\partial x} + v\frac{\partial p}{\partial y}\right)$$

$$\Pi^{(yy)} = \mu\left(2\frac{\partial v}{\partial y} - \left[\frac{2}{3} - \frac{\zeta}{\mu}\right]\operatorname{div}\vec{u}\right) + \tau\gamma p \operatorname{div}\vec{u} + \tau\rho v\left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) + \tau\left(u\frac{\partial p}{\partial x} + 2v\frac{\partial p}{\partial y}\right)$$

$$\Pi^{(xy)} = \mu\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) + \tau\rho u\left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial y}\right)$$

$$\Pi^{(yx)} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \tau\rho v\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial x}\right)$$

Viscosity Tensors and Heat Flux

Heat Flux

$$q^{(x)} = -\kappa \frac{\partial T}{\partial x} - u \cdot R$$

$$q^{(y)} = -\kappa \frac{\partial T}{\partial y} - v \cdot R$$

$$R = \tau\rho \frac{1}{\gamma - 1}\left[u \frac{\partial}{\partial x}\left(\frac{p}{\rho}\right) + v \frac{\partial}{\partial y}\left(\frac{p}{\rho}\right)\right] + \tau\rho p\left[u \frac{\partial}{\partial x}\left(\frac{1}{\rho}\right) + v \frac{\partial}{\partial y}\left(\frac{1}{\rho}\right)\right]$$

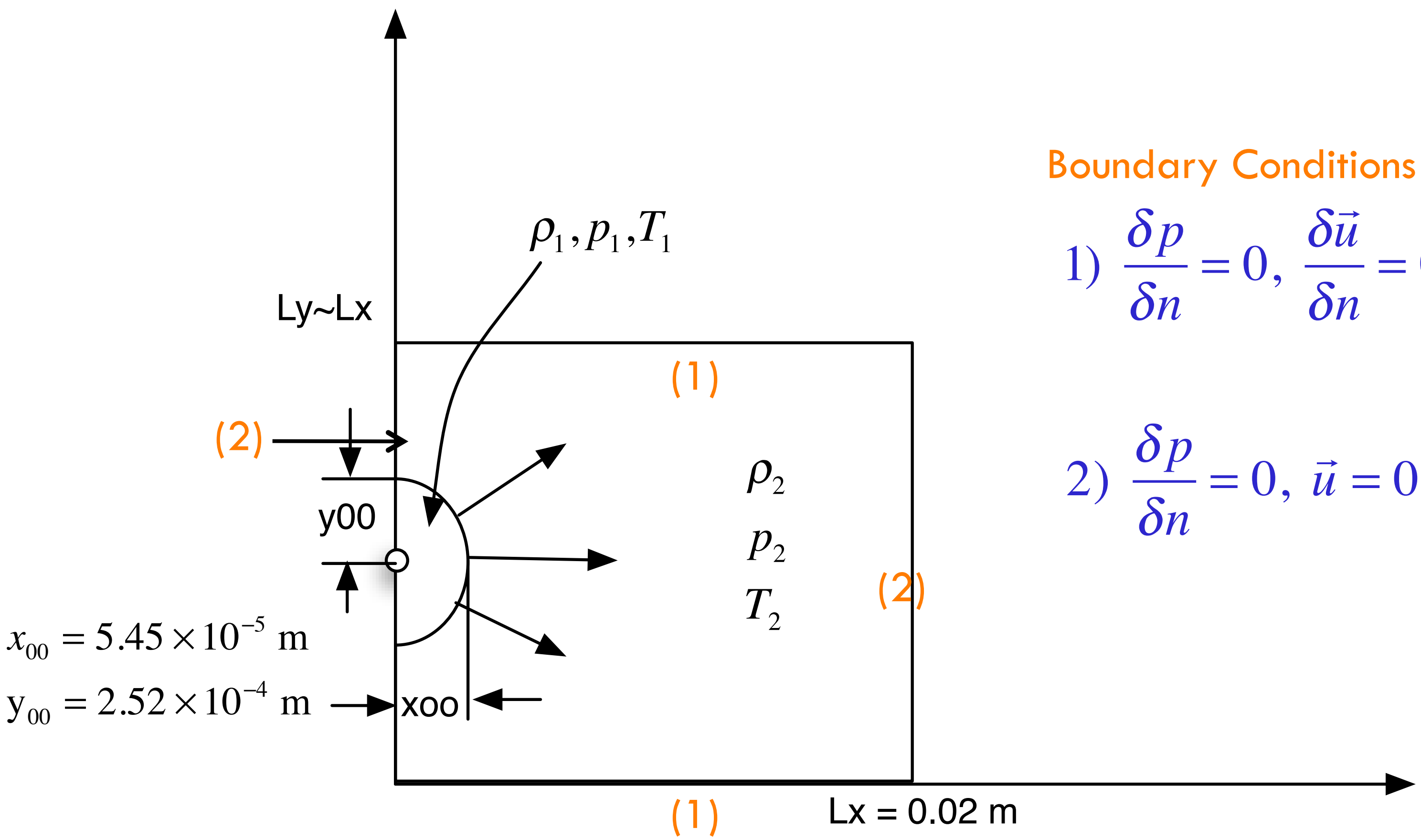
Semi-discrete Form – 2D

$$\frac{d}{dt}\bar{\mathbf{u}}_j(t) = -\frac{\mathbf{H}^x_{j+\frac{1}{2},k}(t) - \mathbf{H}^x_{j-\frac{1}{2},k}(t)}{\Delta x} - \frac{\mathbf{H}^y_{j,k+\frac{1}{2}}(t) - \mathbf{H}^y_{j,k-\frac{1}{2}}(t)}{\Delta y}$$

$$+ \frac{\mathbf{P}^x_{j+\frac{1}{2},k}(t) - \mathbf{P}^x_{j-\frac{1}{2},k}(t)}{\Delta x} + \frac{\mathbf{P}^y_{j,k+\frac{1}{2}}(t) - \mathbf{P}^y_{j,k-\frac{1}{2}}(t)}{\Delta y}$$

1. Hyperbolic Numerical Flux
2. Parabolic Numerical Flux
3. Temporal integration

Initial Conditions
2D Laser Ablation



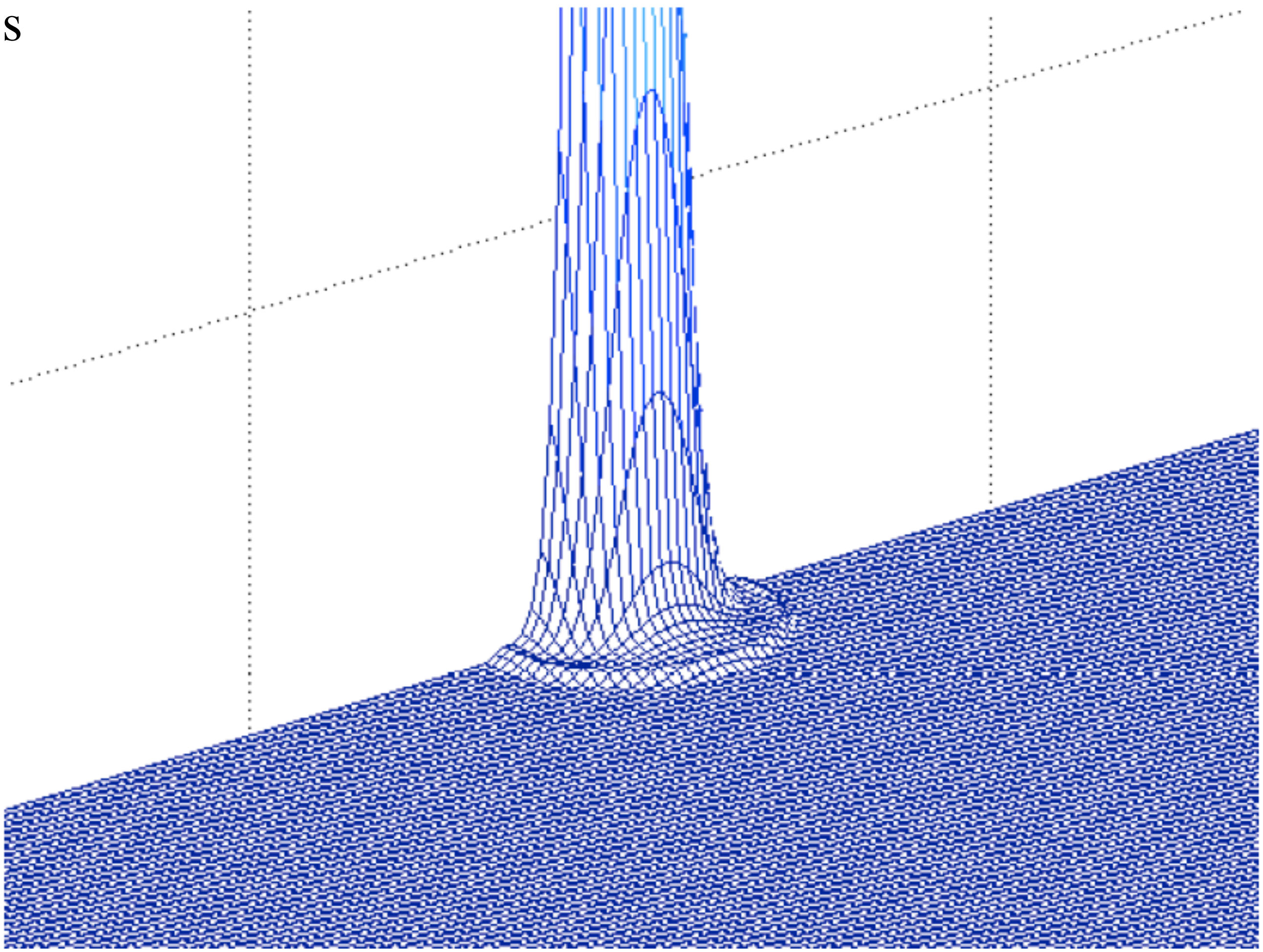
Boundary Conditions

1) $\dfrac{\delta p}{\delta n} = 0, \ \dfrac{\delta \vec{u}}{\delta n} = 0, \ \dfrac{\delta \rho}{\delta n} = 0$

2) $\dfrac{\delta p}{\delta n} = 0, \ \vec{u} = 0, \ \dfrac{\delta \rho}{\delta n} = 0$

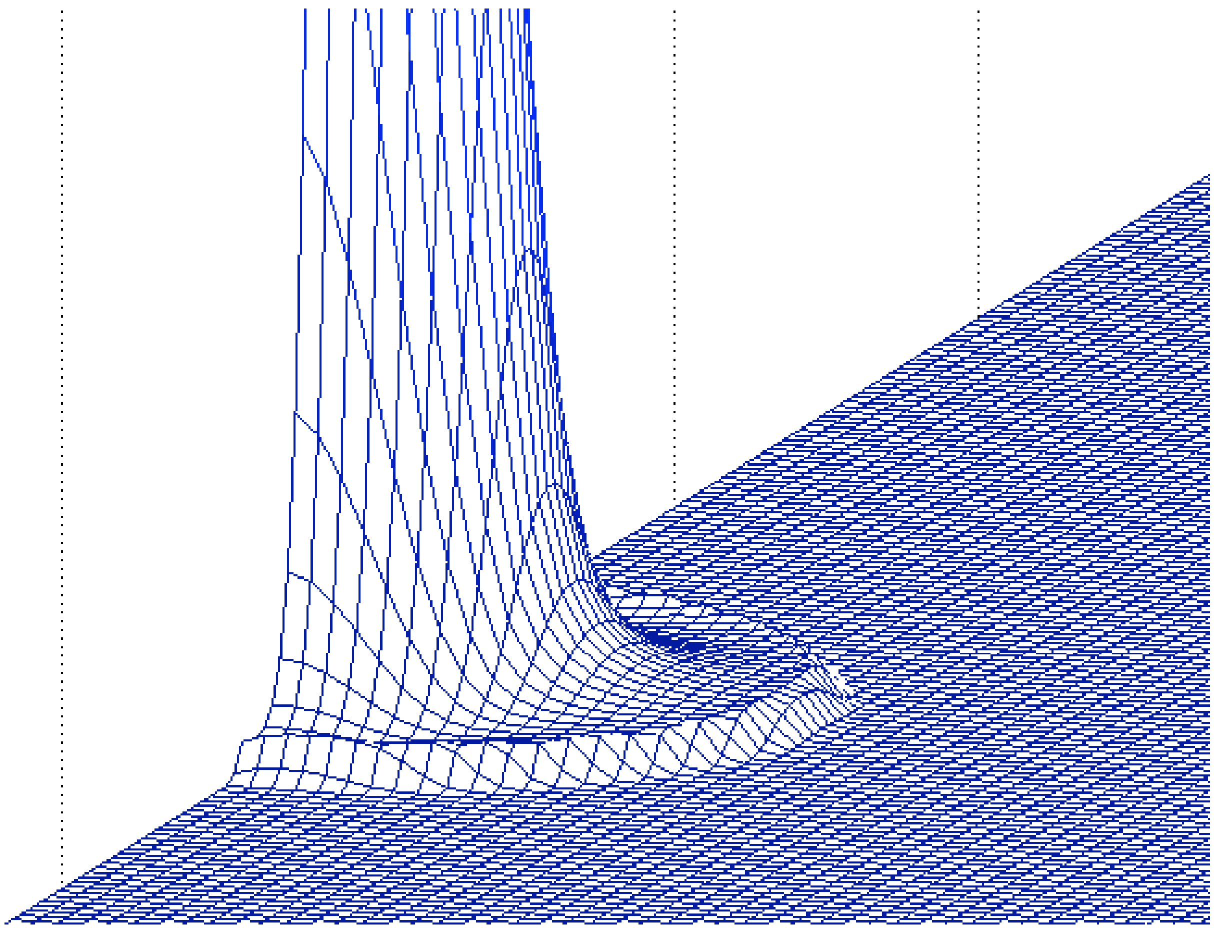
2D QGD Results

$t = 1 \times 10^{-8}$ s



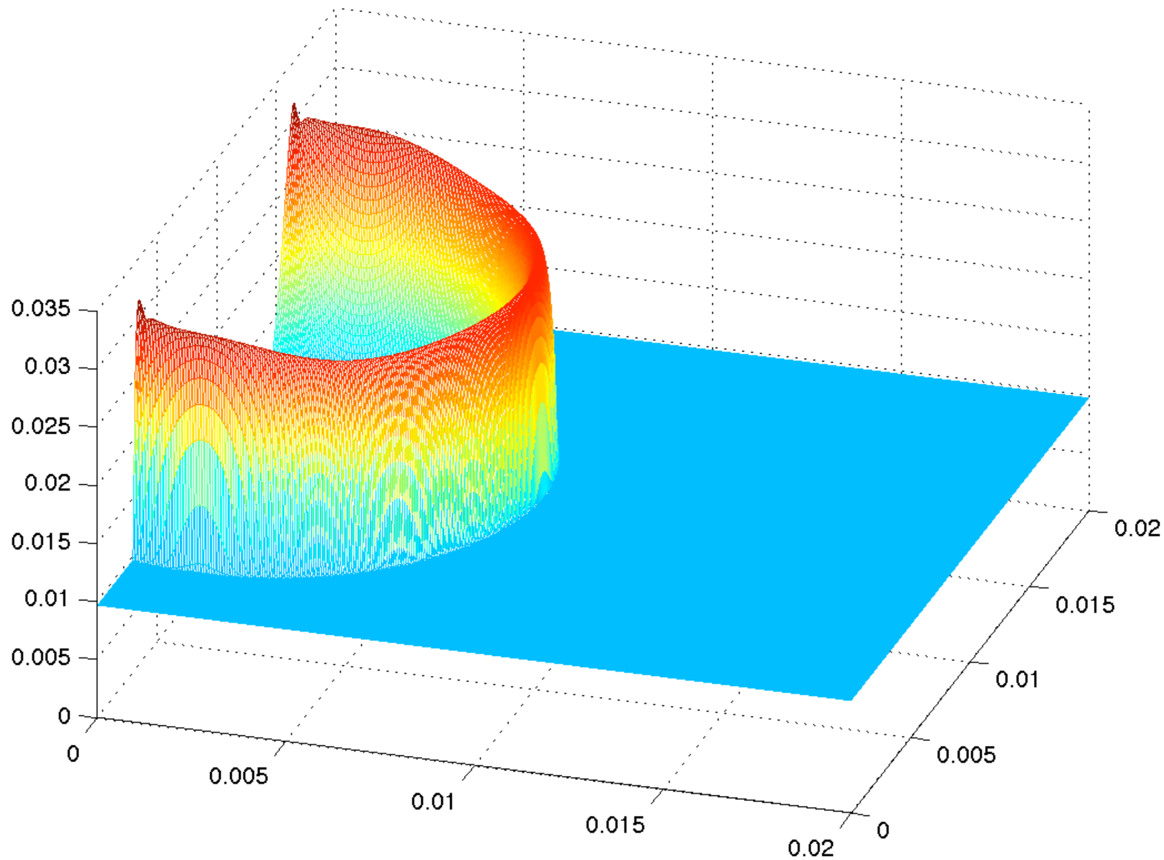
2D QGD Results

$t = 2 \times 10^{-8}$ s



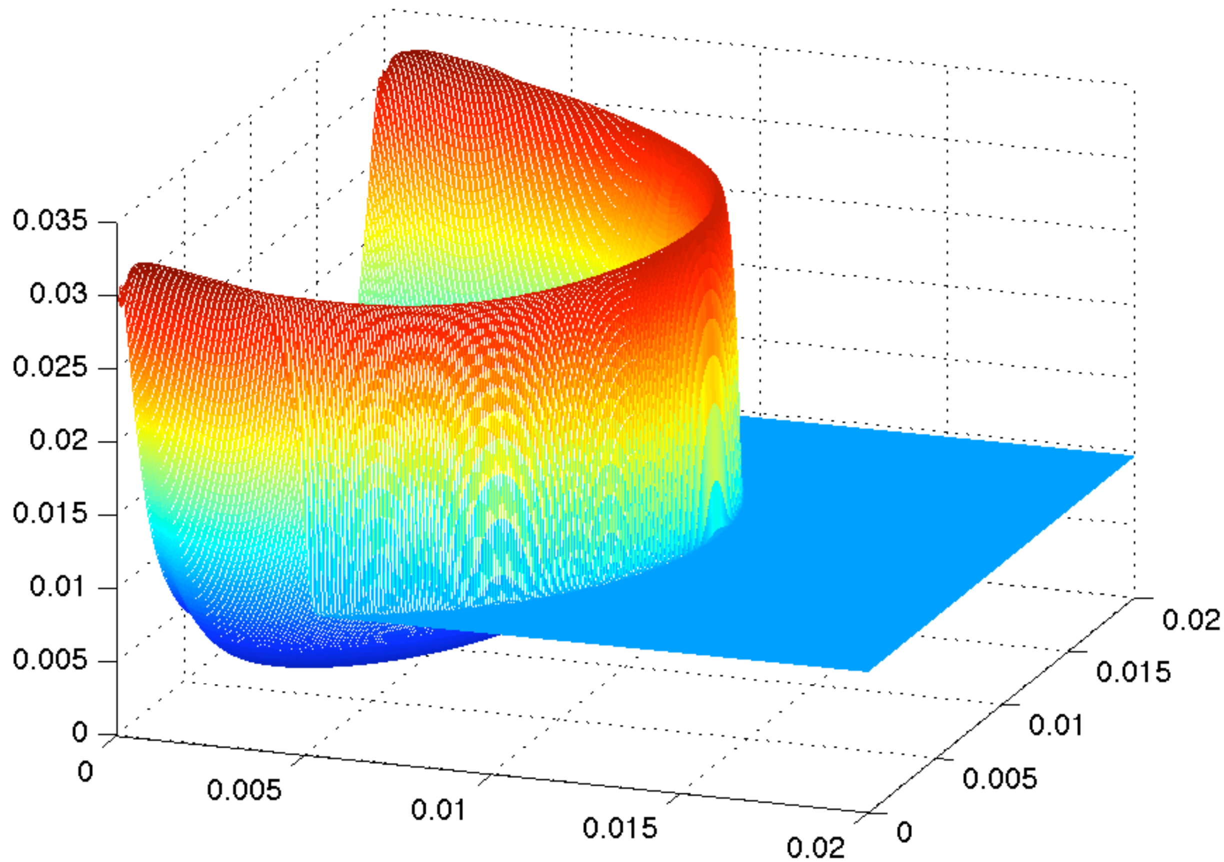
2D QGD Results

$t = 2 \times 10^{-6}$ s



2D QGD Results

$t = 4 \times 10^{-6}$ s



Conclusion

- Decrease cost of computation
- Increase accuracy
- Location of shocks
- Allow for more physically accurate initial conditions
- Apply Navier-Stokes' equations to laser ablation problem
- Computation of the two-dimensional problem

Future Work

- Optimize 2D code
- Investigate the effects of τ on the 2D simulations
- Radially Symmetric simulations
- Expand to three dimensions
  - parallelization
  - radial symmetry

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THANK YOU!